Thermostatted δf

John A. Krommes*
Princeton University, P.O. Box 451, Princeton, New Jersey 08543–0451, USA
(September 23, 1998)

The δf simulation method is revisited. Statistical coarse-graining is used to rigorously derive the equation for the fluctuation δf in the particle distribution. It is argued that completely collisionless simulation is incompatible with the achievement of true statistically steady states with nonzero turbulent fluxes because the variance of the particle weights w grows with time. To ensure such steady states, it is shown that for dynamically collisionless situations a generalized thermostat or "W-stat" may be used in lieu of a full collision operator to absorb the flow of entropy to unresolved fine scales in velocity space. The simplest W-stat can be implemented as a self-consistently determined, time-dependent damping applied to w. A precise kinematic analogy to thermostatted nonequilibrium molecular dynamics (NEMD) is pointed out, and the justification of W-stats for simulations of turbulence is discussed. An extrapolation procedure is proposed such that the long-time, steady-state, collisionless flux can be deduced from several short W-statted runs with large effective collisionality, and a numerical demonstration is given.

PACS: 52.35.Ra, 52.65.Rr

I. INTRODUCTION

The δf simulation method (elaborated upon in Sec. II and Appendix A) is a standard approach to the numerical description of collisionless or nearly collisionless plasmas. However, in a commonly used form of the algorithm the variance W of the marker weights w (which describe the turbulent fluctuations) increases indefinitely in time for collisionless simulations that predict nonzero turbulent flux Γ. (Γ is used here as a generic notation for either particle flux Γ_n or thermal flux Γ_T.) This is troubling for both conceptual and practical reasons. Conceptually, such simulations cannot achieve true statistically steady states (although low-order moments such as the electrostatic potential may saturate), raising the issue of whether a turbulent steady state is, in fact, being simulated. Practically, the indefinite increase of marker variance leads to enhanced noise that eventually limits the effective duration of the simulation. In the present work, I attempt to address these problems. I argue that for collisionless simulations the current algorithm must be augmented to include a *W-stat*, which is a generalized thermostat constructed such that W (or at least its time average) is frozen to a specified value. The W-stat introduces an effective dissipation that balances against the turbulent production of fluctuations (a measure of which is Γ) in just such a way that a true steady state can be achieved. It can be implemented at negligible computational expense by a simple modification to the evolution equation for the weights.

The W-stat is intended to be used for situations that are dynamically collisionless—i.e., those for which the classical Coulomb collision frequency ν is much less than a dynamical mode or eddy-turnover frequency. For completely collisionless dynamics, the δf method is a Monte–Carlo sampling technique in which an ensemble of marker points is integrated along Hamiltonian characteristic trajectories. Such dynamics obey a Liouville theorem in the phase space $\boldsymbol{z} \doteq (\boldsymbol{x}, \boldsymbol{v})$ ($\doteq$ denotes definition). It can be shown that in the presence of turbulence with nonzero flux the marker weights diffuse—i.e., the variance of the weights increases linearly with time. That variance can be related to an appropriate information-theoretic entropy of the turbulence. Introduction of the W-stat deliberately violates Liouville's theorem in the extended phase space $(\boldsymbol{z}, w)$ in such a way that the turbulent diffusion is balanced by an effective dissipation that represents the flow of entropy to unresolved fine scales in velocity space. Of course, dissipative collision operators such as the Landau operator [Eq. (A4)] violate Liouville's theorem as well. The W-stat is an artifice that is intended to replace the complicated details of a collision operator in the limit where those details should not matter.

In order to formulate the W-stat, a precise definition of, and dynamical equation for the marker weights are required. That definition and the theoretical basis for the δf algorithm have been inadequately discussed in the literature, so I will give a systematic reformulation based on statistical averages of the Klimontovich equation, generalizing and unifying techniques first presented in Ref. 1. The derivation emphasizes that the "background" probability density function (PDF) that appears in the familiar decomposition

$$\text{"full } f\text{"} = \text{"background } f\text{"} + \delta f, \tag{1}$$

*E-mail address: `krommes@princeton.edu`.

where the background f is assumed to involve macroscopic, smoothly varying profiles in x or $\boldsymbol{v}$, is the PDF in the *presence* of all turbulent transport effects—an interpretation not in accord with that of most previous workers. The new derivation has the desirable property of maintaining $\langle \delta f \rangle = 0$, where $\langle \ldots \rangle$ is the statistical (ensemble) average.[2] If the algorithm is implemented correctly, spurious long-wavelength fluctuations will not be generated and initial profiles will not relax during the course of a steady-state simulation, as does happen in some extant codes for which $\langle \delta f \rangle \neq 0$.

If the introduction of a W-stat is not to change the value of the simulated turbulent flux Γ, one must show that $\Gamma(W)$ becomes sensibly independent of W for W much greater than a threshold value W_c. That this should be so can be argued both theoretically[3] and from the consistent empirical observation that saturated or quasi-saturated values of Γ are observed in extant collisionless simulations. I will present the results of some preliminary simulations, using a simple two-dimensional (2D) δf code, that support the expected behavior of the W-statted dynamics. Although a number of important and difficult questions remain to be answered, the general conclusion is that for the challenging limit $\nu \to 0$ W-stats may provide viable, computationally inexpensive alternatives to nontrivial numerical implementations of full collision operators; they should be studied further.

The outline of the paper is as follows. In Sec. II I give a careful derivation of a δf algorithm that maintains $\langle \delta f \rangle = 0$. In Sec. III I introduce an appropriate entropy functional and discuss its properties. I describe the derivation, interpretation, and numerical application of an appropriate W-stat in Sec. IV. I discuss the results in Sec. V. In Appendix A I provide additional discussion of both collisionless and collisional δf algorithms. Finally, I devote Appendix B to some technical details relating to entropy and dissipation.

II. REVIEW AND REINTERPRETATION OF THE δf METHOD

In the formulations of the δf method that appear in the literature (for background and historical references, see Refs. 4, 5, and 1), various distribution functions and averaging procedures are frequently confused or specified imprecisely. I therefore give a review and systematic derivation of the δf equation that emphasizes several levels of statistical coarse-graining, the preferred role of the one-particle PDF as a "background" distribution, the importance of maintaining $\langle \delta f \rangle = 0$, and the distinction between the distributions of the physical particles and of the Monte–Carlo markers (sampling points).

A. Statistical averaging, the background PDF, and fluctuations

One considers two classes of particles: (i) the physical ones, whose almost collisionless dynamics are to be simulated (physical distribution functions carry no subscript); (ii) marker particles, used in a Monte–Carlo phase-space sampling technique to implement the δf algorithm (marker distributions and related quantities carry the subscript m; for consistency with other literature,[6] I sometimes write g instead of f_{m}). For either class, there are three levels of description: (i) fully microscopic, described by the singular Klimontovich microdensity $\widehat{f}$ of N_s particles of species s in a volume V (with mean density $\overline{n}_s \doteq N_s/V$):

$$\widehat{f}_s(\boldsymbol{z}, t) \doteq \frac{1}{\overline{n}_s} \sum_{i=1}^{N_s} \delta(\boldsymbol{z} - \widetilde{\boldsymbol{z}}_i(t)), \tag{2}$$

where $\boldsymbol{z}$ denotes the set of phase-space observer coordinates of a single (generic) particle and $\widetilde{\boldsymbol{z}}_i$ denotes the actual (random) trajectory of the ith particle; (ii) a fine-scale average, $\langle \ldots \rangle_{\mathrm{fine}}$, that replaces particle discreteness with a collision operator but leaves macroscopic, collective random fluctuations unaveraged (random fluctuations are indicated by a tilde); (iii) an ensemble average $\langle \ldots \rangle$ over the macroscopic turbulent fluctuations (and over the fine scales as well if that has not already been done). Thus one introduces

$$\widetilde{f} = \langle \widehat{f} \rangle_{\mathrm{fine}}, \quad f = \langle \widetilde{f} \rangle = \langle \widehat{f} \rangle. \tag{3a,b}$$

Equation (3b) is the standard Klimontovich relation between the one-particle PDF[7] f (a smooth function) and the singular microdensity $\widehat{f}$. However, the partially averaged $\widetilde{f}$ (also a smooth function) is often a useful intermediary. The difference between $\widetilde{f}$ and f defines the fluctuation δf (smooth on a microscopic scale but turbulent on a macroscopic scale):

$$\underbrace{\widetilde{f}}_{\mathrm{full}\, f} = \underbrace{f}_{\mathrm{background}} + \underbrace{\delta f}_{\mathrm{fluctuations}}. \tag{4}$$

These definitions are such that δf is a true fluctuation:

$$\langle \delta f \rangle = 0. \tag{5}$$

Virtually all theories of turbulence begin with a decomposition analogous to Eq. (4), with the fluctuations defined relative to the mean field.[8] For spatially homogeneous statistics, Eq. (5) states that δf has no $\boldsymbol{k} = 0$ component. For inhomogeneous statistics, such as occur for global simulations with boundary conditions, profile variations, and/or magnetic shear, the requirement $\langle \delta f \rangle(x) = 0$ means that δf should not develop long-wavelength, time-independent spatial variations.

The distinction between the "background" (statistically averaged) PDF f and the "full distribution" $\widetilde{f}$ is crucial. The smoothly varying mean density or temperature profiles employed in theoretical or experimentally coarse-grained descriptions are properties of the statistically averaged f, not the randomly fluctuating $\widetilde{f}$. When one speaks of a local Maxwellian f_{lM} parametrized by background density $n(x)$ and temperature $T(x)$ with gradients $d\ln n/dx = -\kappa_n$, $d\ln T/dx = -\kappa_T$ (in a global simulation the κ's may depend on x; in local simulations they are usually taken to be constants), one is referring to f; thus

$$d\ln f_{\mathrm{lM}}/dx = -\kappa(\boldsymbol{v}), \tag{6a}$$

where

$$\kappa(\boldsymbol{v}) \doteq \kappa_n + \left(\frac{1}{2}\frac{v^2}{v_{\mathrm{t}}^2} - \frac{3}{2}\right)\kappa_T, \tag{6b}$$

where $v_{\mathrm{t}} \doteq (T/m)^{1/2}$ is the thermal velocity.

In most or all of the previous literature on the δf method, the decomposition $\widetilde{f} = f_0 + \delta f$ has been used, where f_0 is an initial distribution. That is specifically not done in the present work. In the systematic interpretation developed here, f is the *long-time* PDF—in the presence of sources, sinks, and all turbulent transport processes—that would be eventually be achieved by evolution from arbitrary initial conditions. By specifying a time-independent f such as f_{lM}, one commits to studying the properties of a *true steady state* parametrized by a particular value of κ (analogous to calculating the statistical properties of a material at a particular thermodynamic state point). To determine those properties, one is allowed to integrate *infinitely long* if that is necessary to achieve good statistics. Indeed, that integration may be taken even longer than the confinement time of a real device. There is no contradiction with the fact that in reality physical parameters usually evolve on a transport time scale. Thus, steady-state simulations might be used to parametrize fluxes as functions of state point; those parametrizations could then be used in time-dependent transport codes (cf. Ref. 9). Note that the distinction between true steady-state simulations, integrated arbitrarily long, and time-dependent simulations of real devices does not depend on whether the simulation is local (constant κ's, periodic boundary conditions) or global (spanning the whole device, nontrivial boundary conditions at the walls). It is necessary to insist on this in order to counter a frequently-voiced objection that it makes no sense to integrate a global simulation for times longer than a confinement time. That is not correct. It may not be *necessary* to do so, if good asymptotic statistics can be obtained more quickly, but if the simulation algorithm is robust there must be no harm in integrating indefinitely long if a time-independent background is specified, for "steady state" implies the limit $t \to \infty$. It is the fact that collisionless algorithms as currently implemented are not robust in this sense (W increases indefinitely in time) that motivated this work.

Although the present techniques are primarily directed at steady-state simulations, macroscopically time-dependent simulations are possible as well in which $\kappa(\boldsymbol{v}, t)$ or $f(x, \boldsymbol{v}, t)$ are determined self-consistently by evolution on a transport time scale. The important point about the decomposition (4) is that it properly segregates macroscopic profile effects into the background f. In other decompositions, some of those effects can appear in δf, which is confusing on both mathematical and physical grounds.

B. Dynamical equations

The goal is to simulate kinetic (velocity-space-dependent) physics such as described by the electrostatic Klimontovich equation

$$\partial_t \widehat{f} + \boldsymbol{v}\boldsymbol{\cdot}\boldsymbol{\nabla}\widehat{f} + (\widehat{\boldsymbol{E}} + c^{-1}\boldsymbol{v}\times\boldsymbol{B})\boldsymbol{\cdot}\boldsymbol{\partial}\widehat{f} = \widehat{S}. \tag{7}$$

Here $\boldsymbol{\partial} \doteq (q/m)\partial_{\boldsymbol{v}}$, $\widehat{\boldsymbol{E}}$ is to be calculated from Poisson's equation with singular charge determined from $\widehat{f}$, and $\widehat{S}$ is a singular source term for particles and/or heat. Equation (7) contains the effects of both short-wavelength, high-frequency classical collisional processes as well as long-wavelength, low-frequency collective phenomena; the latter are of primary interest here. A fine-scale average of Eq. (7) changes $\widehat{f}$ to $\widetilde{f}$ at the price of adding an appropriate collision term to the right-hand side. A further change of variables to the usual gyrokinetic coordinates[10] then leads to the collisional gyrokinetic equation

$$\frac{D\widetilde{f}}{Dt} = -\widetilde{C}[\widetilde{f}] + \widetilde{S}, \tag{8}$$

where $\widetilde{C}$ is an appropriate collision operator, brackets indicate functional dependence, and

$$\frac{D\widetilde{f}}{Dt} \equiv \frac{\partial\widetilde{f}}{\partial t} + v_\parallel\nabla_\parallel\widetilde{f} + \widetilde{\boldsymbol{V}}_E\boldsymbol{\cdot}\boldsymbol{\nabla}\widetilde{f} + \widetilde{E}_\parallel\partial_\parallel\widetilde{f}. \tag{9}$$

(For simplicity of presentation, the magnetic field is assumed to be constant in space, so gradient and curvature drifts have been omitted. Of course, those drifts can be crucial in practical applications.) I will not be concerned with the detailed form of $\widetilde{C}$ in the body of this paper (see the remarks in Appendix A). However, the mere presence of that dissipative operator will be critical for the later discussion.

In Eq. (9), $\widetilde{\boldsymbol{V}}_E$ and $\widetilde{E}_\parallel$ derive from a fluctuating electrostatic potential $\widetilde{\varphi}$, a macroscopic property of the turbulence.[11] An equation for the usual smooth, positive-semidefinite PDF f emerges by averaging Eq. (8) [or, equivalently, Eq. (7)]. In a geometry in which statistical inhomogeneity is permitted only in the x direction, and with mean fields and the parallel nonlinearity neglected for simplicity, f obeys

$$\partial_t f + \partial_x \mathcal{G} = -\mathcal{C}[f] + S, \tag{10}$$

where the phase-space flux is

$$\mathcal{G}(x, \boldsymbol{v}) \doteq \langle \delta V_{E,x}\, \delta f \rangle \tag{11}$$

and $\mathcal{C}[f] \doteq \langle \widetilde{C}[\widetilde{f}] \rangle$. Velocity moments of $\mathcal{G}$ lead to macroscopically observable fluxes; for example, the particle flux relative to $\overline{n}$ is

$$\Gamma_n(x) \doteq \langle \delta V_{E,x}(\delta n/\overline{n}) \rangle = \int d\boldsymbol{v}\, \mathcal{G}(x, \boldsymbol{v}). \tag{12}$$

(Because of the adopted normalization,[7] one has, for example, $\delta n = \overline{n} \int d\boldsymbol{v}\, \delta f$.) In principle, the solution of Eq. (10), including appropriate sources, sinks, and boundary conditions, defines the background profiles. Clearly those profiles are the ones that develop in the presence of both classical and turbulent transport. The usual procedure of specifying an analytical, time-independent form for f, then solving for δf for fixed f, can be interpreted as obtaining f from experimental measurements of steady-state turbulence rather than from the steady-state solution of Eq. (10).

In full-f simulations, initial conditions are sampled from a given PDF, then integrated along the microscopic Hamiltonian gyrokinetic characteristics. The phase-space density of particles at time t then provides an estimate of $\widetilde{f}(\boldsymbol{z}, t)$. However, that method is noisy; when the fluctuations are small, the full-f algorithm wastes most of its resolution sampling f, which may be an analytically known function such as a local Maxwellian.

In the superior δf method, f is specified and Monte–Carlo sampling[5] is used to resolve just δf. Dealing only with δf leads to a substantial reduction of order $\langle (\delta f/f)^2 \rangle$ in the intensity of the sampling noise.[12,1]

The following discussion is a restatement of material presented in Ref. 1, slightly generalized to include sources and collisions. The rigorous equation for δf is obtained by subtracting Eq. (10) from Eq. (8):

$$\frac{D\delta f}{Dt} = -\underbrace{\delta L\, f}_{1} + \underbrace{\partial_x \mathcal{G}}_{2} - \underbrace{C[\delta f]}_{3} + \underbrace{\delta S}_{4}, \tag{13a}$$

where

$$\delta L \doteq \delta \boldsymbol{V}_E \boldsymbol{\cdot} \boldsymbol{\nabla} + \delta E_\parallel \partial_\parallel \tag{13b}$$

and $C[\delta f] \doteq \widetilde{C}[\widetilde{f}] - \mathcal{C}[f]$. The inhomogeneous equation (13a) contains four distinct kinds of source terms on its right-hand side, which I shall now discuss briefly.

Term 1: x-space or v-space gradients of f. Those can be calculated analytically for simple forms of f; cf. Eq. (6). Thus, for a local Maxwellian the Fourier representation of $\delta L\, f_{\mathrm{lM}}$ is

$$\delta L \, \ln f_{\mathrm{lM}} = -i \left(\frac{T_e}{T_s} \right) \left(\frac{q_s}{e} \right) (\omega_{*s} - k_\parallel v_\parallel) \left(\frac{e\varphi}{T_e} \right), \tag{14}$$

where the diamagnetic frequency is

$$\omega_{*s} \doteq -k_y \left(\frac{cT_s}{q_s B} \right) \kappa(\boldsymbol{v}). \tag{15}$$

Term 2: The divergence of the phase-space flux, $\partial_x \mathcal{G}(x, \boldsymbol{v})$. This term, inherited from Eq. (10), is virtually never written, commented upon, or implemented,[13] presumably because earlier workers have employed different definitions of δf. In the present formalism, it is required in order to ensure that Eq. (13a) preserves $\langle \delta f \rangle = 0$. [The background achieves steady state by a balance between (i) the dissipative effects of the turbulent flux $\mathcal{G}$ (and classical collisions, if present), and (ii) sources and/or boundary conditions.] $\partial_x \mathcal{G}$ vanishes for a local simulation that enforces strict statistical homogeneity in x (constant κ's and periodic boundary conditions). However, it need not vanish for so-called bounded models in which, for example, the potential is set to zero at the simulation boundaries, or more generally for any simulation with inhomogeneous statistics (which includes the practically important cases of magnetic shear and radial profile variations). [For all cases the spatial average (indicated by an overline) of this source term does vanish, $\overline{\partial_x \mathcal{G}} = 0$, provided that δf or $\delta V_{E,x}$ either vanishes at the boundaries or satisfies periodic boundary conditions.]

To the extent that $\partial_x \mathcal{G}$ does not vanish,[13] its absence on the right-hand side of the δf equation can be expected to produce spurious long-wavelength profile relaxation. That is actually observed in global δf simulations,[14] and can partly account for qualitative differences between local and global simulations.

If the parallel nonlinearity is included in the dynamics, the term $\partial_\parallel \langle \delta E_\parallel\, \delta f \rangle$ must be added to $\partial_x \mathcal{G}$. Because there is no translational symmetry in v space, this term does not vanish.

Term 3: A possible collision operator C acting on δf. By definition, this term is omitted for a strictly collisionless simulation. The conventional argument is that C is negligible when the collision frequency is much smaller than the dynamical time scales of the relevant turbulent modes. I will challenge that logic below.

Term 4: A fluctuating source δS. This term is frequently taken to vanish, an experimentally reasonable assumption.[15]

C. Monte–Carlo sampling of Eulerian moments

In the present section I review and discuss conventional algorithms for collisionless δf simulations.

1. Calculation of Eulerian moments

At any time t, Eulerian moments

$$\delta M(\boldsymbol{z}, t) \doteq \int d\overline{\boldsymbol{z}}\, \widehat{M}(\boldsymbol{z}; \overline{\boldsymbol{z}}) \delta f(\overline{\boldsymbol{z}}, t) \tag{16}$$

are required, either for dynamical or diagnostic purposes. (Here M is some moment defined by a specified kernel $\widehat{M}$; a possible species summation is subsumed in the $\overline{z}$ integral.) An example of δM is the fluctuating charge density $\delta\rho$, required for the gyrokinetic Poisson equation, whose kernel is

$$\widehat{\rho}(\boldsymbol{z};\overline{\boldsymbol{z}}) = (\overline{n}q)_{\overline{s}}\delta(\boldsymbol{x}-\overline{\boldsymbol{x}}). \tag{17}$$

Formula (16) defines a phase-space integral that may be evaluated by a variety of techniques. For example, δf might be time-evolved on an Eulerian phase-space grid and (16) evaluated by a Riemann-sum approximation. However, a more conventional choice is to use Monte–Carlo sampling.[5] The Monte–Carlo estimate of an integral

$$I \doteq \int d\boldsymbol{z}\, \widetilde{G}(\boldsymbol{z})K(\boldsymbol{z}), \tag{18a}$$

where K is a given function and $\widetilde{G}$ is a given sampling PDF normalized to unity, is the sample mean (in the usual statistics sense[16])

$$I \approx \langle K\rangle_N \doteq \frac{1}{N_{\rm m}}\sum_{i=1}^{N_{\rm m}} K(\boldsymbol{z}_i). \tag{18b}$$

This formula requires the sampling distribution only at the present time t; it does not depend on the particular, possibly stochastic, way in which the $N_{\rm m}$ sampling points evolved from $t = 0$.

To use Monte–Carlo sampling to estimate formula (16), one may normalize δf to the (smooth) sampling distribution $\widetilde{f}_{\rm m} \equiv \widetilde{g} \doteq V\widetilde{G}$ and define the new field

$$w(\boldsymbol{z}, t) \doteq \delta f(\boldsymbol{z}, t)/\widetilde{g}(\boldsymbol{z}, t). \tag{19}$$

Then

$$\delta M(\boldsymbol{z}, t) = \int d\overline{\boldsymbol{z}}\, \widetilde{g}(\overline{z}, t)\widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})w(\overline{\boldsymbol{z}}, t) \tag{20a}$$

$$\approx \frac{1}{\overline{n}_{\rm m}}\sum_{i=1}^{N_{\rm m}}[\widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})w(\overline{\boldsymbol{z}}, t)]_{|\overline{\boldsymbol{z}}=\tilde{\boldsymbol{z}}_i(t)}. \tag{20b}$$

For specific choices of $\widehat{M}$, it is formula (20b) that is actually implemented in the numerical codes. To coarse-grain δM to an Eulerian grid, say in $\boldsymbol{x}$ space, the sum in Eq. (20b) is merely restricted to the points lying in the appropriate bin (see the discussion of Fig. 8 in Sec. A 1).

Note that Eq. (20b) can be written in terms of a Klimontovich marker distribution $\widehat{f}_{\rm m}$ as

$$\delta M(\boldsymbol{z}, t) \approx \int d\overline{\boldsymbol{z}}\, \widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})w(\overline{\boldsymbol{z}}, t)\widehat{f}_{\rm m}(\overline{\boldsymbol{z}}, t) \tag{21a}$$

$$= \int d\overline{\boldsymbol{z}}\, \widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})\delta\widehat{f}_{\rm m}(\overline{\boldsymbol{z}}, t), \tag{21b}$$

where the effective sampling distribution is

$$\delta\widehat{f}_{\rm m}(\boldsymbol{z}, t) \doteq \frac{1}{\overline{n}_{\rm m}}\sum_{i=1}^{N_{\rm m}} w_i\delta(\boldsymbol{z}-\widetilde{\boldsymbol{z}}_i(t)). \tag{22}$$

Because of the appearance of the w_i's in the Klimontovich-like expression (22), the w's are frequently called the "particle weights." However, this use of "particle" is unfortunate; as will be emphasized below, the marker distribution differs in general from the true particle PDF that is being simulated. The w's should more appropriately be called the "sampling weights" or the "marker weights"; I shall simply call them the "weights."

The singular sampling distribution (22) is convenient for theoretical calculations of statistical sampling noise.[1] However, it must not be confused with the smooth function δf. The goal of the simulation is to calculate δf; the discrete collection of markers is merely introduced as a means to that end.

The problem is now reduced to the evaluation of the weights at the time-evolved positions of the markers. Thus, at time $t = 0$ $N_{\rm m}$ points are sampled from some prescribed marker distribution $f_{\rm m}$. (That distribution may be unrelated to the initial condition on δf.) Those points are allowed to evolve according to prescribed equations of motion, which in principle may be quite arbitrary. Given those equations (which may include stochastic elements such as random parallel accelerations or perpendicular velocities; see the discussion in Sec. A 2), the Liouville equation for the sampling distribution can be determined theoretically. The δf equation is already known [cf. Eq. (13a)], so from the definition (19) the evolution equation for w is fully determined. This conclusion differs from the recent assertion of Chen and White,[6] who suggested that in the presence of stochastic scattering of the marker trajectories it was necessary to introduce an extended phase space in which w played the role of an independent variable. Although that may provide a theoretically elegant reformulation, it is unnecessary; the sampling distribution $\widetilde{g}$ exists and obeys a definite equation of motion even in the presence of stochastic scattering. To emphasize this point, in Sec. A 2 I rederive the algorithm of Chen and White directly from the definition (19).

It is now clear that markers are distinct from physical particles: They may evolve from different initial conditions, possibly in the presence of different sources, and they may even obey different equations of motion.

Although the marker trajectories may be arbitrary in principle, in certain situations advantages accrue to specific choices. In particular, in collisionless theory it is useful to require the markers to obey the same characteristic trajectories as do the physical particles. (That still does not imply that $\widetilde{f}_{\rm m} = \widetilde{f}$, since the initial conditions and sources may differ for the physical and marker distributions.) In the presence of collisions, that is not possible. Markers are true test particles; they are introduced as an artifice to aid in the solution of the specified

δf equation, and cannot react back on the dynamics of δf in any way. Physical particles, on the other hand, are not true test particles. A given particle polarizes the sea of all other particles; that effect is responsible for frictional drag and the momentum and energy conservation laws of the Balescu–Lenard and Landau collision operators. However, it is useful to assume that the marker characteristics are the physical ones determined by collisionless dynamics, plus an as-yet unspecified stochastic part related to collisions. Then, upon coarse-graining over the stochastic element, one has [cf. Eq. (8)]

$$\frac{D\widetilde{f}_{\mathrm{m}}}{Dt} = -\widetilde{C}_{\mathrm{m}}[\widetilde{f}_{\mathrm{m}}] + \widetilde{S}_{\mathrm{m}}, \tag{23}$$

where the marker collision operator $\widetilde{C}_{\mathrm{m}}$, implicitly dependent on $\widetilde{f}$, is unspecified at this point.

2. Evolution of the weights

The equation for w follows by substituting $\delta f = w\widetilde{f}_{\mathrm{m}}$ into Eq. (13a). In organizing and simplifying the result, the quantity[1]

$$p(\boldsymbol{z},t) \doteq f(\boldsymbol{z},t)/\widetilde{f}_{\mathrm{m}}(\boldsymbol{z},t) \tag{24}$$

enters naturally because one wants to refer quantities to f in order to exploit the given properties of the background, as in Eq. (6). With the aid of Eq. (23), one obtains

$$\frac{Dw}{Dt} = p\{-\delta L \ln f + f^{-1}[\partial_x \mathcal{G} + (\delta S - \delta C) - w(\widetilde{S}_{\mathrm{m}} - \widetilde{C}_{\mathrm{m}})]\}. \tag{25}$$

Equation (25) is a partial differential equation for the Eulerian field $w(\boldsymbol{z},t)$. However, if the markers are chosen to obey the characteristic equations of motion of the physical particles, Eq. (25) becomes an ordinary differential equation for the weight $w_i(t)$ integrated along the ith trajectory:

$$\frac{dw_i}{dt} = R_i(t) \equiv R(\widetilde{\boldsymbol{z}}_i(t),t), \tag{26}$$

where $R(\boldsymbol{z},t)$ is the right-hand side of Eq. (25).

To obtain a dynamical equation for p, note, from the definitions (24) and (19), that

$$p + w = (f + \delta f)/\widetilde{f}_{\mathrm{m}} = \widetilde{f}/\widetilde{f}_{\mathrm{m}}. \tag{27}$$

Hence

$$\frac{D(p+w)}{Dt} = \frac{1}{\widetilde{f}_{\mathrm{m}}}\frac{D\widetilde{f}}{Dt} - \frac{\widetilde{f}}{\widetilde{f}_{\mathrm{m}}^2}\frac{D\widetilde{f}_{\mathrm{m}}}{Dt} \tag{28a}$$

$$= \widetilde{f}_{\mathrm{m}}^{-1}[(\widetilde{S} - \widetilde{C}) - (p+w)(\widetilde{S}_{\mathrm{m}} - \widetilde{C}_{\mathrm{m}})]. \tag{28b}$$

In the absence of both sources and collisional (discreteness) effects, Eq. (28b) shows that $p + w$ is conserved along the Lagrangian trajectories:

$$p_i(t) + w_i(t) = p_i(0) + w_i(0) \doteq c_i, \tag{29}$$

where the c_i's are constants. In that case, if one chooses to load the markers in the same way as is done for the actual particles, one has $p(0) + w(0) = \widetilde{f}(0)/\widetilde{f}_{\mathrm{m}}(0) = 1$, hence $p_i(t) = 1 - w_i(t)$; this recovers the "fully nonlinear" scheme of Parker and Lee.[4] It must be emphasized that this is not the only possibility. For example, in a local simulation the markers could be loaded uniformly in space, whereas f would typically be assumed to contain a weak profile gradient and $\delta f(0)$ might be initialized to a small sinusoidal perturbation. For such initializations, $\widetilde{f} \neq \widetilde{f}_{\mathrm{m}}$, the relative difference being of the order of κL_x (L_x being the x dimension of the simulation box) and δf.

The difference between c_i and unity can be large. As an example, let the background f be a local Maxwellian with density and temperature profiles characterized by the inverse scale lengths κ_n and κ_T, and let the initial marker distribution be Maxwellian in velocity but uniform in space (this initialization scheme is used frequently in practice). Then, upon normalizing velocities to v_{t}, one finds

$$c(x,\boldsymbol{v}) = \exp\bigl(-[\kappa_n + (\tfrac{1}{2}v^2 - \tfrac{3}{2})\kappa_T]x\bigr). \tag{30}$$

For positive κ's, the maximum value of c is attained for $v = 0$:

$$c_{\max}(x) = \exp\bigl(-(\kappa_n - \tfrac{3}{2}\kappa_T)x\bigr) \approx \exp(\tfrac{3}{2}\kappa_T x), \tag{31}$$

the last approximation holding for the usual case of ion-temperature-gradient-driven (ITG) fluctuations with $\eta \doteq \kappa_T/\kappa_n \gg 1$. Although in a local simulation one would typically have $\overline{L} \doteq \kappa_T L_x < 1$, so that $c_{\max}$ would not differ substantially from unity, realistic global simulations may well require $\overline{L} > 1$; for $\overline{L} = 2$, $c_{\max} \approx 20$. A scatter plot of c for the above assumptions is shown in Fig. 1. (The upper boundary is associated with zero-velocity particles. Points close to $c = 0$ stem from superthermal particles.) Another way of quantifying the size of c is to average it over the marker PDF. For a Maxwellian distribution, the velocity integral can be performed analytically, leading to

$$\overline{C}(\overline{L};\eta) = \langle c \rangle_{x,\boldsymbol{v}} = \frac{1}{\overline{L}}\int_0^{\overline{L}} d\overline{x}\, \frac{\exp\bigl((3/2 - \eta^{-1})\overline{x}\bigr)}{(1+\overline{x})^{3/2}}. \tag{32}$$

This function is graphed in Fig. 2.

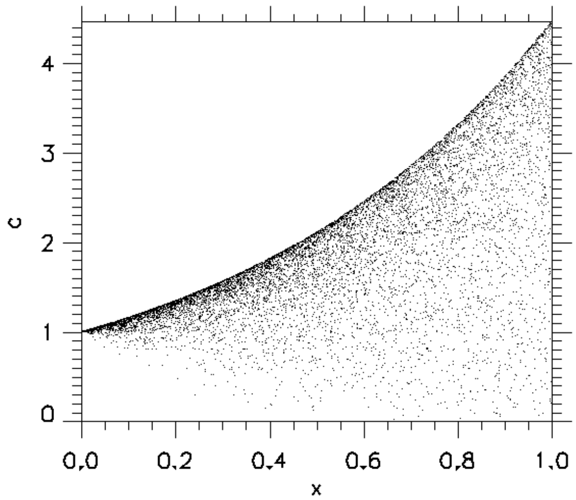

FIG. 1. Representative distribution of $c \doteq p(0) + w(0)$ for a marker distribution of 10 000 points uniform in space and Maxwellian in velocity. $\overline{L} = 1$ and $\eta = \infty$.

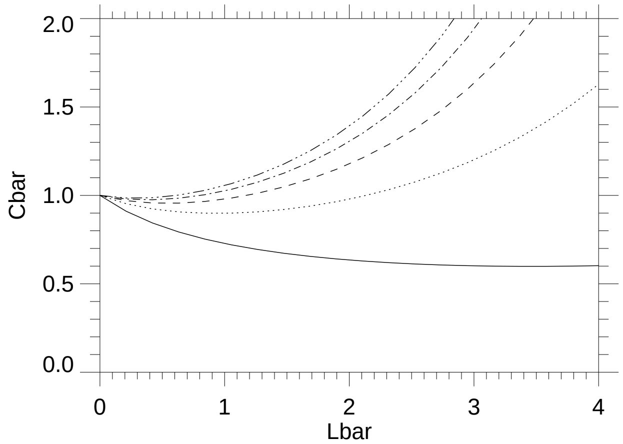

FIG. 2. The function $\overline{C}(\overline{L}; \eta)$ defined by Eq. (32). The curves correspond, from bottom to top, to $\eta = \{1, 2, 3, 4, 5\}$.

In the absence of sources and collisions, there would appear at first glance to be no technical reason why the general result

$$p_i(t) = c_i - w_i(t) \tag{33}$$

should not be used for arbitrary marker loadings. The term c_i is simply a time-independent N-dimensional vector that is fully determined by the initial loading scheme and is trivial to implement in the computer codes. However, preliminary experiments with this algorithm for cases where $\overline{C}(\overline{L}, \eta) - 1 \geq \mathcal{O}(1)$ have not been entirely successful. One question is how to treat markers that diffuse to $w_i \sim c_i$. Such markers, even if relatively few, can contribute anomalously large statistical noise that contaminates the measurements. In preliminary experiments with very long runs using Eq. (33), I have sometimes observed cases of spontaneous symmetry breaking in which $\langle w \rangle$, whose time average should vanish due to number conservation (see the next section), instead suddenly rises from noise and saturates close to $\overline{C}$. Fortunately, the W-statting technique described in Sec. IV works with small w's and relatively short times.

3. Number conservation

In the absence of physical sources, the total number of particles is conserved. For steady state, the mean density is time-independent, so one focuses on the density fluctuation δn. From

$$0 = V^{-1} \int d\boldsymbol{x}\, \frac{\delta n}{\overline{n}} \tag{34a}$$

$$\approx V^{-1} \int d\boldsymbol{x} \int d\overline{\boldsymbol{z}}\, \delta(\boldsymbol{x} - \overline{\boldsymbol{x}}) \delta\widehat{f}_{\mathrm{m}} \tag{34b}$$

$$= \frac{1}{N_{\mathrm{m}}} \sum_{i=1}^{N_{\mathrm{m}}} w_i, \tag{34c}$$

one concludes that, at any time t, the sum of the weights [the sample mean $\langle w \rangle_N(t)$] should vanish. From Eq. (26), number conservation is preserved if $\langle R \rangle_N = 0$. That will not be true if cavalier approximations are made for p.

To demonstrate the consistency of the exact formulation, consider how the sample mean of the first term on the right-hand side of Eq. (25) vanishes. One has

$$p\, \delta L\, \ln f = \widetilde{f}_{\mathrm{m}}^{-1} (\delta \boldsymbol{V}_E \boldsymbol{\cdot} \boldsymbol{\nabla} + \delta E_\parallel \partial_\parallel) f; \tag{35}$$

upon referring to Eqs. (18), one has

$$\langle p\, \delta L \ln f \rangle_N \approx \frac{1}{V} \int d\boldsymbol{z}\, \widetilde{f}_{\mathrm{m}}\, p\, \delta L \ln f \tag{36a}$$

$$\approx \frac{1}{V} \int d\boldsymbol{z}\, [\boldsymbol{\nabla \cdot} (\delta \boldsymbol{V}_E f) + \partial_\parallel (\delta E_\parallel f)]_i \tag{36b}$$

$$= 0 \tag{36c}$$

(the last integrand being a perfect derivative). The same argument shows that the $\partial_x \mathcal{G}$ term integrates away.

Of course, this argument ignores statistical sampling errors; in practice, $\langle w \rangle_N$ will fluctuate randomly. Although mild fluctuations around $\langle w \rangle_N = 0$ may not be important, there can be troubling secular effects. In particular, inconsistent values or dynamics for p can easily lead to violation of number conservation.

The approximation $p \approx 1$ and uniform marker loading preserves number conservation by expression (35), but for a reason different than the general calculations of Eqs. (36). Consider just the $\boldsymbol{E} \times \boldsymbol{B}$ term for simplicity. Then for $p = 1$

$$p\, \delta \boldsymbol{V}_E \boldsymbol{\cdot} \boldsymbol{\nabla} \ln f \to -\kappa\, \delta V_{E,x}. \tag{37}$$

For a uniform initial marker distribution, spatial homogeneity is preserved under the time evolution, so the markers remain uniformly distributed in space. Then

$$\langle p\,\delta\boldsymbol{V}_E\boldsymbol{\cdot}\boldsymbol{\nabla}\ln f\rangle_N = \frac{1}{N}\sum_i(-\kappa\,\delta V_{E,x}) \tag{38a}$$

$$\propto \int d\boldsymbol{x}\,\delta V_{E,x} = 0, \tag{38b}$$

the last result following since $\delta V_{E,x} \propto -\partial\delta\varphi/\partial y$ (or, more generally, by virtue of an ergodicity argument that equates spatial and ensemble averages).

This concludes the systematic derivation of the collisionless δf algorithm. I have stressed (i) the presence of the $\partial_x\mathcal{G}$ term for inhomogeneous simulations, and (ii) the necessity of a consistent treatment of the second weight p. These points are frequently not dealt with correctly in the extant codes, and further research is required to bring their implementation to a satisfactory state. Additional remarks on collisionless δf are given in Appendix A 1, where the role of the Lagrangian phase-space lattice is discussed.

In addition to the technical details discussed in this section, there remains a crucial conceptual problem with the collisionless algorithm in its present form. Namely, it can be shown that *collisional dissipation is never negligible* even in the limit of vanishing collision frequency. This is related to the so-called *entropy paradox*[3] discussed in the next section.

III. ENTROPY EVOLUTION AND δf

The role of collisional dissipation is best understood from the point of view of information-theoretic entropy. For some background discussion and references, see Ref. 3.

A. Information-theoretic entropy

In addition to the ensemble average $\langle\ldots\rangle$ already introduced, it is convenient to define a barring operation on an arbitrary random function $A(\boldsymbol{z})$ by

$$\overline{A} \doteq V^{-1}\int d\boldsymbol{z}\,f(\boldsymbol{z})\langle A(\boldsymbol{z})\rangle. \tag{39}$$

(f plays the role of a weight function in a scalar product defined globally on the phase space.) Then the information-theoretic entropy relative to the background PDF f and coarse-grained over the fine scales is[17,3]

$$\overline{\mathcal{S}} = -\overline{\left(\frac{\widetilde{f}}{f}\right)\ln\left(\frac{\widetilde{f}}{f}\right)} \tag{40a}$$

$$= -V^{-1}\int d\boldsymbol{z}\,\langle\widetilde{f}\ln(\widetilde{f}/f)\rangle. \tag{40b}$$

As discussed in Ref. 3, processes that drive $\widetilde{f}$ away from f (e.g., turbulent production or flux) tend to *reduce* $\overline{\mathcal{S}}$ (make it more negative), whereas ones that relax $\widetilde{f}$ toward f (e.g., collisional dissipation) tend to *increase* $\overline{\mathcal{S}}$ (drive it toward zero). Through second order in δf, one has

$$\overline{\mathcal{S}} \approx -\frac{1}{2}\overline{(\delta f/f)^2}. \tag{41}$$

B. Production, dissipation, and the entropy paradox

It is useful to define the positive-definite functional $\overline{\mathcal{F}} \doteq -\overline{\mathcal{S}}$; then

$$\overline{\mathcal{F}} = \frac{1}{2}\overline{(\delta f/f)^2} = \frac{1}{2}V^{-1}\int d\boldsymbol{z}\,\langle\delta f^2\rangle/f. \tag{42a,b}$$

Early numerical studies of this functional were made in Ref. 18. In addition to its interpretation in terms of entropy, $\overline{\mathcal{F}}$ is a convenient measure of phase-space fluctuation intensity. As discussed with a variety of examples in Ref. 3, a generic equation for $\overline{\mathcal{F}}$ is

$$\partial_t\overline{\mathcal{F}} = \overline{\mathcal{P}} - \overline{\mathcal{D}}, \tag{43}$$

where $\overline{\mathcal{P}}$ represents the turbulent production of fluctuations and $\overline{\mathcal{D}}$ is the collisional dissipation (not, it must be stressed, collisionless dissipation due to Landau damping[1]). Such balance equations are very familiar in the theory of neutral fluids; cf. Ref. 19. They also arise naturally in the theory of variational bounds on transport.[20,21]

In Ref. 3, it was stressed that collisional dissipation cannot be ignored if a statistically steady state is to be achieved. That is clear from Eq. (43), for if $\overline{\mathcal{D}}$ is neglected, then

$$\overline{\mathcal{F}}(t) - \overline{\mathcal{F}}(0) = \int_0^t dt'\,\overline{\mathcal{P}}(t') \sim \overline{\mathcal{P}}(\infty)t \tag{44a,b}$$

for $t > \tau_{\rm ac}$, $\tau_{\rm ac}$ being the Lagrangian correlation time of the turbulence such that $\overline{\mathcal{P}}$ attains its asymptotic steady-state value $\overline{\mathcal{P}}(\infty)$ for $t > \tau_{\rm ac}$. It was this general behavior that in Ref. 3 was named the *entropy paradox*: a statistical observable ($\overline{\mathcal{F}}$) is changing in time in a purported steady state, so a true steady state cannot, in fact, have been achieved. The necessity of including some sort of real dissipation even in situations in which the nonlinear dynamics are essentially collisionless will lead me in the next section to a discussion of W-stats.

It is instructive to rewrite Eq. (42b) in terms of w and p. Upon appropriately multiplying and dividing by $\widetilde{f}_{\rm m}$, one finds $\overline{\mathcal{F}} = \langle\widetilde{\mathcal{F}}\rangle$, where

$$\widetilde{\mathcal{F}} = \frac{1}{2}V^{-1}\int d\boldsymbol{z}\,\widetilde{f}_{\rm m}(w^2/p) \approx \frac{1}{2}\langle w^2/p\rangle_N, \tag{45a,b}$$

where Eqs. (18) were used. Essentially (to the extent that $p \approx 1$), $\mathcal{F}$ is half of the mean-squared weights.

There is a striking and precise analogy between formula (45b) for $\widetilde{\mathcal{F}}$ and the instantaneous mean kinetic energy $\widetilde{\mathcal{K}}$—i.e., the kinetic temperature T—of a many-body system:

$$\widetilde{\mathcal{K}} = \frac{1}{2}\langle \boldsymbol{p}^2/m\rangle_N, \tag{46}$$

where $\boldsymbol{p}_i$ is the canonical momentum and m_i is the mass of the ith particle. Clearly

$$w \sim \boldsymbol{p}, \quad p \sim m. \tag{47a,b}$$

This analogy will be exploited in the discussion of W-stats in Sec. IV.

C. Illustration: The Langevin–Fokker–Planck model

To understand the relation between Eq. (25) (for the evolution of the weights) and Eq. (43) (the generic equation for entropy evolution), consider the simplified model

$$\dot{w} = \kappa\, \delta V_{E,x} - f^{-1}C[\delta f]. \tag{48}$$

I have approximated $p \approx 1$ ($\widetilde{f}_{\mathrm{m}} \approx f$), ignored parallel effects, spatial inhomogeneity, sources, and marker discreteness. The approximation $p \equiv 1$ can never be precisely correct, because $\widetilde{f}_{\mathrm{m}}$ is a random variable whereas f is not; however, Eq. (48) captures the essence of the dynamical effects and balances of present concern. For definiteness, I illustrate with the Langevin–Fokker–Planck operator (physically appropriate for ion–electron collisions)

$$C[\delta f] = -\frac{\partial}{\partial v}\left(\nu v + D_v \frac{\partial}{\partial v}\right)\delta f, \tag{49}$$

where $v \equiv v_\parallel$ and the velocity-space diffusion coefficient is related to ν *via* the Einstein relation $D_v = v_{\mathrm{t}}^2\nu$. This operator is linear and annihilates a Maxwellian distribution, so it is appropriate to take f to be Maxwellian in velocity space. Then (still ignoring the precise distinction between $\widetilde{f}_{\mathrm{m}}$ and f),

$$C[\delta f] \approx C[wf] = -D_v \frac{\partial}{\partial v}\left(f\frac{\partial w}{\partial v}\right). \tag{50}$$

The collisional contribution to $\overline{\mathcal{F}} = \frac{1}{2}V^{-1}\int d\boldsymbol{z}\,\langle \delta f^2\rangle/f$ is

$$\partial_t \overline{\mathcal{F}}_{\mathrm{coll}} = -V^{-1}\int d\boldsymbol{z}\,\langle(\delta f/f)C[\delta f]\rangle \tag{51a}$$

$$= D_v V^{-1}\int d\boldsymbol{z}\left\langle w\frac{\partial}{\partial v}\left(f\frac{\partial w}{\partial v}\right)\right\rangle \tag{51b}$$

$$= -\overline{\mathcal{D}}, \tag{51c}$$

where

$$\mathcal{D} \doteq D_v\left\langle\left(\frac{\partial w}{\partial v}\right)^2\right\rangle. \tag{52}$$

The contribution of turbulent scattering to $\dot{\mathcal{F}}$ is

$$\frac{d}{dt}(\frac{1}{2}\langle w^2\rangle) = \langle \dot{w}(t)\, w(t)\rangle \tag{53a}$$

$$= \langle \kappa\, \delta V_{E,x}(t)\int_0^t dt'\, \kappa\, \delta V_{E,x}(t')\rangle \tag{53b}$$

$$\approx \kappa^2 D, \tag{53c}$$

where $D \doteq \int_0^\infty d\tau\,\langle \delta V_{E,x}(\tau)\delta V_{E,x}(0)\rangle$ is the turbulent particle diffusion coefficient, the time integral of the Lagrangian velocity correlation function. [For simplicity, collisions were ignored in writing Eq. (53b); that is not fundamental, and a more precise calculation can be done.[3]] Thus one recovers Eq. (43) with $\Gamma = \kappa D$ (the usual Fick's law for turbulent diffusion) and $\mathcal{D}$ given by Eq. (52). Again, note that to the extent that the turbulent flux is nonzero, $\overline{\mathcal{F}}$ grows without bound when the collision operator is set to zero:

$$\overline{\mathcal{F}}(t) - \overline{\mathcal{F}}(0) \to (\kappa\overline{\Gamma})t \quad (t > \tau_{\mathrm{ac}},\ C \equiv 0). \tag{54}$$

D. The origin of the small velocity scales

As was shown in Ref. 3, a consequence of Eq. (54) is that if one is interested in true statistically steady states in which healthy, nonzero turbulent fluxes flow, it is never correct to study collisionless dynamics; dissipation remains nonzero as $\nu \to 0$. This is a consequence of the fact that the nonlinear dynamics generate finer and finer velocity-space scales for which the collisional effects are enhanced. When the nonlinear dynamics are essentially collisionless (meaning that the collision frequency is much less than the dynamical frequencies), the dissipation scale in v space is *determined* by the nonlinear dynamics in just such a way that collisional dissipation balances with turbulent production. There is a precise analogy[3] to the energy cascade in three-dimensional Navier–Stokes turbulence, in which the Kolmogorov dissipation microscale is determined as a function of the Reynolds number based on the macroscopic velocity and spatial scale.

The most obvious mechanism for generating small scales in velocity space is the nonlinear stretching associated with the parallel acceleration problem $\dot{z} = v_\parallel$, $\dot{v}_\parallel = (q/m)E_\parallel$. In unmagnetized theory, that is the only possibility. However, in strongly magnetized situations dominated by $\boldsymbol{E}\times\boldsymbol{B}$ drifts, the parallel nonlinearity is usually small and is frequently neglected. It might then seem that the velocity derivatives in dissipation functionals such as (52) would remain bounded as $t \to \infty$, in which case $\overline{\mathcal{D}}$ would vanish with ν. That is not correct, however; velocity derivatives can be amplified indirectly by *spatial* diffusion, as I now discuss.

That velocity and spatial derivatives are linked in the presence of collisional dissipation in a plasma is an old and elementary idea familiar to all students of the Chapman–Enskog solution of Landau's kinetic equation for the classical plasma transport coefficients.[22] Basically, the velocity-space distortion of the first-order distribution from a Maxwellian is proportional to spatial gradients of the fluid quantities, so when fine spatial scales are generated by any means, the velocity derivative of δf grows. Small spatial scales can be generated by the Hamiltonian stretching associated with $\boldsymbol{E}\times\boldsymbol{B}$ motion (cf. the 2D enstrophy cascade), or by nonlinear mode coupling from perpendicular to parallel directions. It is those nonlinear spatial processes, not the parallel nonlinearity, that drive the collisional dissipation in typical tokamak microinstability problems.

For a specific model, I consider in Appendix B the Chapman–Enskog solution for the PDF of a Brownian test particle. Such a particle obeys the diffusion equation

$$\frac{\partial}{\partial t}\left(\frac{\delta n}{\overline{n}}\right) = D\frac{\partial^2}{\partial x^2}\left(\frac{\delta n}{\overline{n}}\right), \tag{55}$$

and the collisional contribution to the evolution of a fluid information–theoretic entropy $\overline{\mathcal{N}} \doteq \frac{1}{2}\overline{(\delta n/\overline{n})^2}$ is $\partial_t\overline{\mathcal{N}} = -\overline{\mathcal{D}}$, where

$$\overline{\mathcal{D}} \doteq D\overline{\left[\frac{\partial}{\partial x}\left(\frac{\delta n}{\overline{n}}\right)\right]^2}. \tag{56}$$

The calculations in Appendix B show in quantitative detail how formula (56), which manifestly involves spatial derivatives, is essentially equal to formula (52), which involves velocity derivatives.

IV. W-STATTED δf

That collisional dissipation is always important in guaranteeing statistically steady states poses something of a problem for particle simulation. In principle, it is possible to simulate the actual plasma collision operator. One such scheme for δf simulations has been given recently by Chen and White[6] (who cite earlier work on this topic); see the discussion in Sec. A 2. If the details of the collision process [for example, either the magnitude or the velocity dependence of $\nu(v)$] are important, some such detailed modelling would appear to be the only option. However, it is nontrivial to implement the full operator, and when one wishes to pass to the limit $\nu \to 0$ that approach may be either unnecessary or impractical.[23] Instead, a W-stat may be useful.

A. Thermostats in nonequilibrium molecular dynamics

A W-stat is a generalization of the thermostat that has long been used in homogeneous nonequilibrium molecular dynamics (NEMD) simulations[24] to stabilize the kinetic temperature [Eq. (46)]. In homogeneous NEMD, one begins by inventing a fictitious external force that interacts with the particles (in a generally non-Newtonian way) and drives, say, a heat flux. The interaction law is chosen in such a way that the driven flux agrees with the theoretical prediction of linear response theory.[25] However, such driving heats the system, which therefore does not remain at a fixed thermodynamic state point. Measurements made on such time-dependent systems are difficult to interpret. Of course, if the particles were in contact with a heat bath in the usual sense of equilibrium statistical mechanics, net heating would not occur. However, in the homogeneous simulations particle–wall interactions are not modelled explicitly and the N simulation particles form a closed system. In the absence of the thermal drive, energy rather than temperature is conserved; the particle distribution is microcanonical, not canonical.

In modern NEMD applications, these difficulties are overcome by using thermostats to effectively place the N simulation particles in contact with a heat bath. They are generally implemented as a simple time-dependent Langevin-like damping in the momentum equation:

$$\dot{\boldsymbol{p}}_i = \boldsymbol{F}_i - \widetilde{\zeta}(t)\boldsymbol{p}_i. \tag{57}$$

Here $\widetilde{\zeta}$ is the thermostat and $\boldsymbol{F}$ represents the total forces on the particles (both internal and external, Newtonian and fictitious). The value of $\widetilde{\zeta}$ is determined from appropriate sums over all particles, so $\widetilde{\zeta}$ carries no i subscript. (For consistency with previous notation, $\boldsymbol{p}_i$ and $\boldsymbol{F}_i$ should also be marked with a tilde, but that is omitted here to reduce clutter.) In the so-called Gaussian[26] isokinetic thermostat, $\widetilde{\zeta}$ is constructed to hold the kinetic temperature precisely constant. Thus, upon noting that $\dot{\widetilde{\mathcal{K}}} = N^{-1}\sum_i \dot{\boldsymbol{p}}_i\boldsymbol{\cdot}\boldsymbol{p}_i/m_i$, one can multiply Eq. (57) by $\boldsymbol{p}_i/m_i$ and sum over all particles to obtain

$$\dot{\widetilde{\mathcal{K}}} = 0 = \left(N^{-1}\sum_i \boldsymbol{F}_i\boldsymbol{\cdot}\boldsymbol{p}_i/m_i\right) - \widetilde{\zeta}\left(N^{-1}\sum_i \boldsymbol{p}_i^2/m_i\right). \tag{58}$$

This determines $\widetilde{\zeta}$, at each time step, to be

$$\widetilde{\zeta} = \frac{\langle \boldsymbol{F}\boldsymbol{\cdot}\boldsymbol{p}/m\rangle_N}{2\mathcal{K}}, \tag{59}$$

where $\mathcal{K} = \widetilde{\mathcal{K}}$ is constant. Alternatively, a differential equation for $\widetilde{\zeta}$ can be given such that merely the time average of $\mathcal{K}$ is held constant. The standard choice here is the Nosé–Hoover thermostat,[27,25] which implements an integral feedback.[28]

The thermostat models the flow of heat from the thermally driven system to a heat bath; it allows a true steady state to develop. By direct analogy, a W-stat may be used to model the flow of entropy from the plasma system (driven by profile and/or velocity gradients) to the unresolved fine scales in velocity space. If an actual collision operator is not implemented, then a W-stat or similar device *must* be; otherwise a true statistically steady state with nonzero turbulent flux cannot be achieved.

B. The Gaussian W-stat

A first attempt at a W-statted version of the model equation (48) (generalized to $p \neq 1$) is

$$\dot{w}_i = p_i(\kappa \mathcal{V}_i - \widetilde{\zeta} w_i), \tag{60a}$$

$$\dot{p}_i = -\dot{w}_i, \tag{60b}$$

where I use $\mathcal{V} = \delta V_{E,x}$ for notational simplicity. (Parallel effects can be incorporated simply by generalizing the definition of $\mathcal{V}$. Possible generalizations of the Krook-like damping term $-\widetilde{\zeta} w$ will be discussed in Sec. IV D.) A Gaussian W-stat that holds $\widetilde{W} \doteq N^{-1} \sum_i w_i^2/p_i$ precisely constant can be constructed by noting that

$$\frac{d}{dt}(\frac{1}{2}w^2/p) = (w/p)\dot{w} - \frac{1}{2}(w^2/p^2)\dot{p} \tag{61a}$$

$$= \left(\frac{wc'}{p^2}\right)\dot{w}, \tag{61b}$$

where

$$c' \doteq p + \frac{1}{2}w = c - \frac{1}{2}w \tag{62}$$

[see Eq. (29)]. Thus, upon multiplying Eq. (60) by $(wc'/p^2)_i$ and summing over i, one finds

$$\widetilde{\zeta} = \kappa \widetilde{\Gamma}'/\widetilde{W}', \tag{63}$$

where

$$\widetilde{\Gamma}' \doteq N^{-1} \sum_i (\mathcal{V} wc'/p)_i, \tag{64a}$$

$$\widetilde{W}' \doteq N^{-1} \sum_i (w^2 c'/p)_i; \tag{64b}$$

the primes denote the presence of the factors c'/p and $W = \widetilde{W}$ is held constant by the Gaussian W-stat. If c'/p is approximated by 1 ($c \approx 1$, $w \ll 1$), $\widetilde{\Gamma}' \to \widetilde{\Gamma}$ (the instantaneous particle flux as measured in the simulation) and $\widetilde{W}' \to \widetilde{W}$. Factors analogous to c'/p do not appear in the NEMD expression (59) because the particle mass is independent of time, whereas p is not. Note that $\widetilde{\zeta}$ fluctuates in time (being a ratio of sample means).

A physical interpretation of $\widetilde{\zeta}$ follows by replacing $\kappa\widetilde{\Gamma}$ in Eq. (63) by the known steady-state dissipation $\mathcal{D}$ that is being modelled; from Eq. (52), the steady-state balance $\overline{\mathcal{P}} = \overline{\mathcal{D}}$ [see Eq. (43)], and the Einstein relation between D_v and ν, one obtains

$$\overline{\zeta} = \langle \widetilde{\zeta} \rangle = D_v \overline{\left\langle \left(\frac{\partial w}{\partial v}\right)^2 \right\rangle} / W \sim \nu \left(\frac{v_{\mathrm{t}}}{\delta v}\right)^2 \doteq \nu_{\mathrm{eff}}. \tag{65}$$

Here δv is, by definition, the *Taylor* microscale[29,30,3] in velocity space (*not* the Kolmogorov velocity dissipation microscale). $\overline{\zeta}$ is thus an effective collision frequency or scattering rate based on the Taylor microscale. According to Eq. (B9), an alternative form is

$$v_{\mathrm{t}}/\delta v = \lambda_{\mathrm{mfp}}/\delta x, \tag{66}$$

δx being Taylor's classical spatial microscale.

Another insight into the interpretation of the W-stat comes from considering the Liouville equation for W-statted particle dynamics in the extended space $(\{\boldsymbol{z}\}, \{w\})$, where the braces indicate the set of coordinates for all of the N particles:

$$\frac{\partial}{\partial t} P(\{\boldsymbol{z}\}, \{w\}, t) + \sum_i \left[\frac{\partial}{\partial \boldsymbol{z}_i} \boldsymbol{\cdot} (\dot{\boldsymbol{z}}_i P) + \frac{\partial}{\partial w_i}(\dot{w}_i P)\right] = 0. \tag{67}$$

Although the flow is incompressible in the usual $\boldsymbol{z}$ space ($\partial_{\boldsymbol{z}} \boldsymbol{\cdot} \dot{\boldsymbol{z}} = 0$), it is compressible in the w direction:

$$\frac{\partial \dot{w}_i}{\partial w_i} \approx -\zeta < 0, \tag{68}$$

where an unimportant term $\partial\zeta/\partial w_i$ of $\mathcal{O}(1/N)$ has been omitted for clarity. That is, the W-stat causes phase-space volumes to contract in the w direction, consistent with its interpretation as modelling the dissipative effects of the unresolved degrees of freedom.

Some discussion of the relationship of the W-stat to the full plasma collision operator is given in Sec. A 2.

C. Justification of the W-stat for simulations of turbulence

To this point, the analogy between thermostatted NEMD and W-statted δf has been precise. However, the procedures for calculating the steady-state flux differ substantially. In NEMD, the thermodynamic state point (the temperature, in particular) is fixed by the thermostat, and the simulation is run until the thermal flux Q saturates; the saturated value of Q is the desired answer. In turbulent δf, however, the effective state point (namely, the value of the steady-state entropy, or equivalently of W) is not known in advance, but in principle must be computed by a complete solution to the turbulence problem (in the presence of collisions). W-statted δf will produce a steady-state flux for any W, but only one of those W's is the physical one that corresponds to the balance between turbulent production and collisional dissipation in a saturated state. A conventional collisional simulation would be run as an initial-value problem until that balance was achieved; however, in the limit of weak collisions the required run time may be prohibitive. In the present method, by contrast, the steady-state version of Eq. (43) is asserted for all times. (This does not mean that the value of $\overline{\Gamma}$ is time-independent. There will be a short initial transient of approximate duration $\tau_{\rm ac}$ during which phase correlations are built up from the random initial conditions. However, each step in that process corresponds to the same W, which means that one avoids a possibly long initial phase during which the weights themselves build up to their natural level.)

1. *An extrapolation procedure for the collisionless flux*

To determine the appropriate W to use in parametrizing the steady state, it is necessary to understand the statistical behavior of the Langevin equation (60). Let us assume that $\mathcal{V}$ is a random variable characterized by a Lagrangian autocorrelation time $\tau_{\rm ac}$, and that $\zeta \equiv \nu_{\rm eff}$ is constant. Then Eq. (60) is identical to the model equation (119) analyzed in great detail in Ref. 3. Consider in particular the physical limit $\nu_{\rm eff}\tau_{\rm ac} \ll 1$. Then it was shown in Ref. 3 that, although the flux asymptotes to the constant value $\Gamma_\infty \to \kappa D$ on the short $\tau_{\rm ac}$ scale, the entropy has singular behavior that depends on the order of the limits $t \to \infty$ and $\nu_{\rm eff} \to 0$:

$$W(t) = \kappa^2 D \left(\frac{1 - e^{-2\nu_{\rm eff} t}}{2\nu_{\rm eff}} \right) \tag{69a}$$

$$\to \begin{cases} \kappa^2 D / 2\nu_{\rm eff} & (\nu_{\rm eff} t \to \infty), \\ \kappa^2 D t & (\nu_{\rm eff} t \to 0). \end{cases} \tag{69b}$$

The limit $\nu_{\rm eff} t \to 0$ recovers Eq. (54); the physical limit, however, is fixed, nonzero $\nu_{\rm eff}$ and $\nu_{\rm eff} t \to \infty$.

This behavior may be exploited to determine the physical flux in W-statted δf. Thus, one expects that in the physical dynamics with real collisional dissipation, to the extent that $\nu_{\rm eff}\tau_{\rm ac} \ll 1$ the flux should quickly saturate on the $\tau_{\rm ac}$ time scale while $W(t)$ should saturate only on the longer (effective) collisional time scale. This temporal behavior of the real dynamics of a single (possibly long) run can be transcribed to the behavior of a series of (relatively short) steady-state W-statted runs parametrized[31] by W. That is, $\Gamma(W)$ should become asymptotically independent of W for $W > W(\tau_{\rm ac})$. Thus, an extrapolation procedure is suggested in which $\Gamma(W)$ is computed (with the W-statted dynamics) for an appropriate range of relatively small W. (Small W corresponds to large effective dissipation.) If the results indicate a sensible trend toward asymptotic independence as W increases ($\nu_{\rm eff}$ decreases), the curve can be extrapolated to the limit $W \to \infty$; the physical flux is $\Gamma(\infty)$. Notice that this procedure, depicted in Fig. 3, neither requires nor produces the actual physical value of $W(t = \infty)$, which according to Eq. (69b) is finite, not infinite.

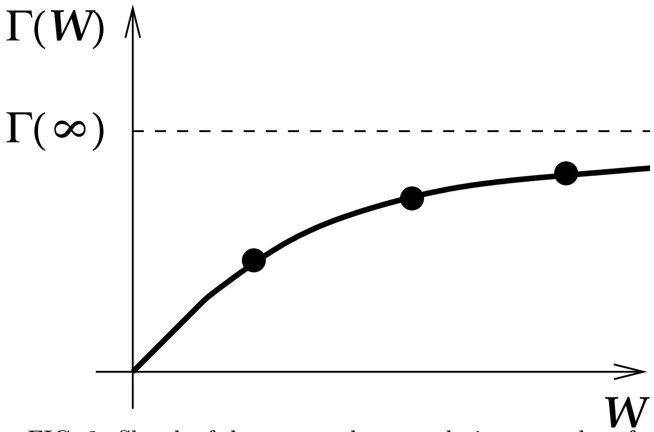

FIG. 3. Sketch of the proposed extrapolation procedure for inferring the asymptotic steady-state flux Γ. Solid line is fit to the several data points; $\Gamma(\infty)$ is the limit of that fit as $W \to \infty$. In the physical state with nonzero collisionality, $W(t = \infty)$ is finite.

2. *Numerical demonstration*

I have performed preliminary numerical experiments to test the feasibility of these ideas. I employed a 2D, unsheared-slab, gyrokinetic simulation code,[32] versions of which have been used frequently in the past to analyze microinstabilities and develop simulation techniques. Although the dynamics evolve in two dimensions, parallel motion and Landau damping are included by setting $k_z = \theta k_y$, $\theta \ll 1$. ITG fluctuations are simulated by imposing adiabatic electron response.

The Fourier amplitudes $(k_x, k_y, k_z) = (k_x, 0, 0)$ ["$(0,0)$ modes"] have special importance. They correspond to random potentials that vary only in the x direction, hence generate random shear flows (zonal flows) in the y direction. In modern simulations of toroidal microinstabilities, substantial evidence has accrued suggesting that such modes can dramatically affect and suppress the overall level of the turbulence. In slab geometry they are driven entirely nonlinearly, since all linear terms in the gyrokinetic operator involve either k_y or k_z [cf. Eq. (14)]. Toroidal effects are thus important to a proper description, but they are still a subject of active research this article. In the present unsheared-slab simulations it appears that the fundamental mode $(1, 0, 0)$ does not saturate, possibly a consequence of negative eddy viscosity. Therefore, in the runs reported here the potentials $\varphi_{k_x,0,0}$ were clamped to zero during the solution of the gyrokinetic Poisson equation, following a long-standing practice for this 2D model. Note that the goal of the present numerical experiments is not to perform realistic simulations of confined plasmas but to compare some basic properties of thermostatted and non-thermostatted simulations; for that purpose, this simple model suffices.

The basic code as provided by previous authors[32] implemented a bounded model in which the potential was clamped to zero at $x = 0$ and $x = L_x$ by employing a Fourier sine transform. That is convenient for generalization to magnetic shear and arbitrary profiles, but introduces a weak translational inhomogeneity that can complicate the interpretation. For periodic boundary conditions, which I have also implemented and studied, statistical invariance under translation (κ = constant) ensures that the flux $\mathcal{G}(x, \boldsymbol{v})$ is rigorously independent of x [see the discussion after Eq. (15)]. The model that was actually studied omitted the $\partial_x \mathcal{G}$ term (as well as sources and explicit collisions) on the right-hand side of Eq. (13a) for both kinds of boundary conditions; that is, the weight equation was the first line of Eq. (25). No qualitative differences were observed between runs with different boundary conditions.

As mentioned at the end of Sec. II C 2, runs with $p = c - w$ encountered fluctuation difficulties that have not yet been fully resolved, so the runs reported here used $p = 1$. All of the runs used a grid of $(n_x, n_y) = (32, 64)$ cells and 25 000 particles, corresponding to about 12 particles per Eulerian spatial cell. Box lengths of $(L_x, L_y) = (32, 64)$ (in units of ρ_s) were used. For the bounded model, those correspond to fundamental wave numbers (mode spacings) of $(\pi/L_x, 2\pi/L_y) \approx (0.1, 0.1)$, and to maximum k's approximately equal to 3 in each direction. I used the parameters $\kappa_n = 0$, $\kappa_T = 0.03$, and $\theta = 0.006$, which according to numerical solution of the linear slab ITG dispersion relation positions the linearly most unstable mode at $(k_x, k_y) \approx (0, 0.5)$.

The relatively small numbers of particles and modes, necessary for rapid real-time turnaround in this exploratory phase, mean that instantaneous flux measurements exhibit considerable noise. In modern 3D simulations that use millions of particles and many modes, that noise is considerably reduced. Nevertheless, qualitative differences have been observed between thermostatted and unthermostatted runs.

In Fig. 4 is shown the thermal flux Γ_T for a typical unthermostatted simulation that grows from noise; the corresponding evolution of $W \doteq \langle \delta w^2 \rangle_N$ is shown in Fig. 5. Γ_T is observed to saturate around $t \approx 5 \times 10^3$, and the mean-square weights W are seen to grow linearly with time. However, increased noise on the flux is observed as W grows beyond 0.2. The run was terminated shortly after that point, partly because of the enhanced noise, partly because the basic approximation $w \ll 1$ was breaking down.

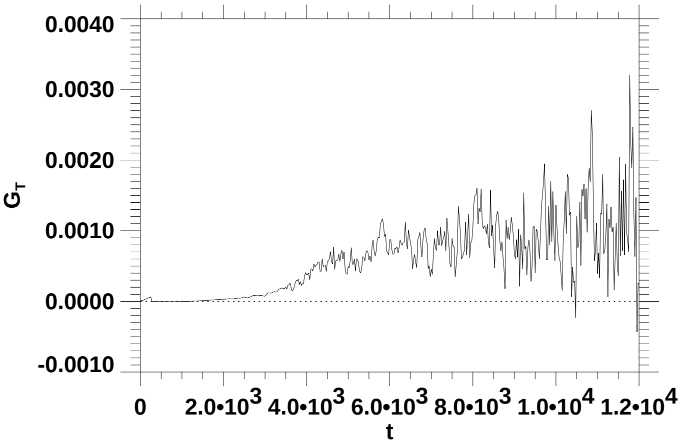

FIG. 4. Typical Γ_T for unthermostatted simulation. See text for parameters.

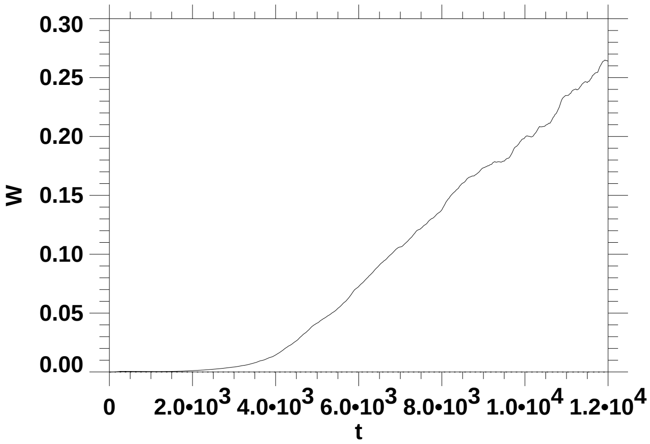

FIG. 5. $W(t)$ corresponding to Fig. 4.

The Gaussian thermostat $-\zeta w$ can be implemented with a minimum of complication. In the original unthermostatted version of the code (a second-order predictor–corrector in time), a single loop was used for both correcting the particle coordinates and weights and accumulating diagnostics. Because ζ depends on the current values of the fluxes, it was necessary to split that loop into two: the first corrects the coordinates and accumulates the fluxes (using the predicted weights); the second corrects w using the new ζ. Such modifications involve only a few lines of code. More accurate algorithms are also feasible.

To test the extrapolation procedure, thermostatted runs were performed for $W \in \{0.0125, 0.025, 0.05, 0.1, 0.15, 0.2\}$. In practice, the numerical algorithm does not clamp W precisely to its specified initial value. To compensate for that (small) error, the weights were renormalized at each time step to have zero average and the specified W; although that procedure is almost certainly unnecessary, it eliminated one possible source of confusion in interpreting the results. The flux for $W = 0.05$ is shown in Fig. 6. Note that (i) the flux rises quickly to its saturated value; (ii) the simulation has been run much longer (measured from the onset of saturation) than the unthermostatted one shown in Fig. 4, yet the noise level does not grow; (iii) the time-averaged flux is lower than in Fig. 4 (this value of W is moderately dissipative). The steady-state fluxes extracted from the indicated runs are plotted in Fig. 7; they are seen to exhibit the qualitative W dependence suggested in Fig. 3. Also shown in Fig. 7 is the least-squares fit to the function

$$\Gamma(W) = \frac{aW}{1+bW}, \tag{70}$$

dependent on the two parameter a and b. This form is motivated by the analytical solution of the model problem in Ref. 3; it is seen to provide a quite reasonable description of the data. With this form, the extrapolated collisionless flux is

$$\Gamma(\infty) = a/b, \tag{71}$$

which for this particular data evaluates to $\Gamma(\infty) \approx 0.00126$. This is somewhat higher than, but in not unreasonable agreement with the later stages of the unthermostatted flux.

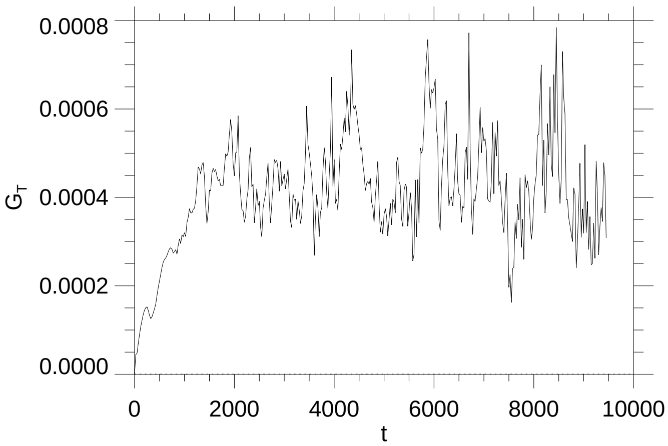

FIG. 6. Representative thermal flux for a thermostatted run; $W = 0.05$. Note the vertical scale change from Fig. 4; thermostatted runs have significantly reduced fluctuations.

It should be noted that, for the purposes of Fig. 7, determination of the steady-state flux was done by a relatively crude time-averaging procedure that could be refined. The fitting process could also be improved by incorporating the experimental uncertainties into the relative weighting of the data points. However, for this initial qualitative demonstration such refinements did not seem warranted.

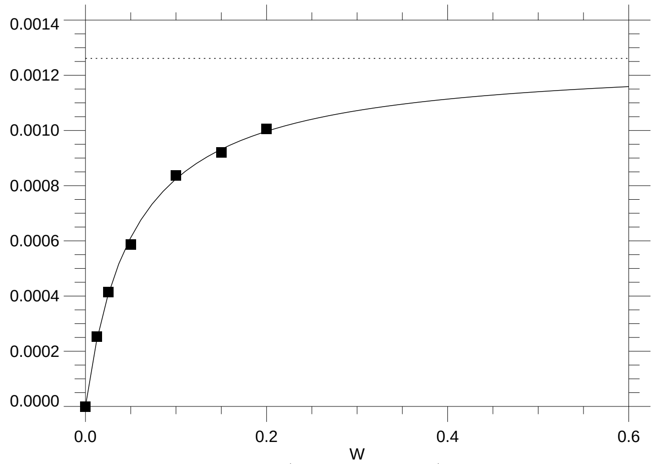

FIG. 7. Data points (solid squares) from a series of thermostatted runs, and fit (solid line) to the function $\Gamma(W) = aW/(1+bW)$. The dotted line indicates the asymptotic value $\Gamma(\infty) = a/b$.

D. W-statting, conservation laws, and shear-flow modes

At first glance, one might be tempted to identify the thermostatting term $-\zeta w$ with a simple Krook model $-\nu\delta f$ of a collision operator. That interpretation is incorrect in two (related) ways: (i) a Krook model would usually involve the actual collision frequency ν, whereas it has been shown that $\zeta \sim \nu_{\mathrm{eff}} \gg \nu$; (ii) the Krook model is linear (ν is independent of the turbulence level), whereas thermostatting is nonlinear (ζ is proportional to Γ and, hence, to the turbulence level). Nevertheless, simple Krook-like operators do not properly respect the conservation laws of the true collision operator. A term $-\zeta w$ is essentially equivalent to a damping $-\zeta\delta f$ in the equation for $\partial_t \delta f$; such damping conserves neither number, momentum, nor kinetic energy.[33]

To rectify this problem, one can apply the W-stat not to δf, but rather to $\mathsf{Q}\delta f$. Here Q is a projection operator defined by $\mathsf{Q} \doteq \mathsf{I} - \mathsf{P}$, where I is the unit tensor and P projects into the null eigenspace of the collision operator. This is consistent with the idea that in steady state low-order fluid moments quickly saturate and do not contribute to the time evolution of $\overline{\mathcal{F}}$. Thus, introduce a Dirac notation and scalar product in velocity space[34] such that $|\, a\,\rangle \equiv af$, $\langle\, a\,| \equiv a$, $\langle a \mid b\rangle \doteq \int d\boldsymbol{v}\, a(\boldsymbol{v})b(\boldsymbol{v})f(\boldsymbol{v})$ (a species summation is omitted for simplicity), and write $\delta f = \delta\chi f = |\,\delta\chi\,\rangle$. Then, upon noting that $|\,\delta\chi\,\rangle = (\mathsf{P}+\mathsf{Q})|\,\delta\chi\,\rangle$ and that P and Q are orthogonal, one has

$$2\overline{\mathcal{F}} = \overline{(\delta f/f)^2} \tag{72a}$$

$$= \overline{\langle\, (\mathsf{P}+\mathsf{Q})\delta\chi \mid (\mathsf{P}+\mathsf{Q})\delta\chi\,\rangle} \tag{72b}$$

$$= \overline{\langle\, \delta\chi \mid (\mathsf{P}^2+\mathsf{Q}^2) \mid \delta\chi\,\rangle} \tag{72c}$$

$$= \overline{\langle \|\mathsf{P}\delta\chi\|^2\rangle} + \overline{\langle \|\mathsf{Q}\delta\chi\|^2\rangle}; \tag{72d}$$

for times $t > \tau_{\rm ac}$, only the Q term contributes to $\dot{\overline{\mathcal{F}}}$.

The simplest example of this general discussion is to define P to extract the density fluctuations from δf. Then

$$\delta n/\overline{n} = \langle\, 1 \mid \delta\chi\,\rangle, \tag{73}$$

and the projection operator that extracts the relative density fluctuation is $\mathsf{P} = |\,1\,\rangle\langle\,1\,|$; hence

$$\mathsf{Q}|\,\delta\chi\,\rangle = (\mathsf{I} - |\,1\,\rangle\langle\,1\,|)|\,\delta\chi\,\rangle = |\,\frac{\delta f}{f}\,\rangle - \frac{\delta n}{\overline{n}}|\,1\,\rangle. \tag{74}$$

Since

$$\delta f - \frac{\delta n}{\overline{n}} f = \widetilde{f}_{\rm m}\left[w - p\left(\frac{\delta n}{\overline{n}}\right)\right], \tag{75}$$

one is led to replace the W-stat term $-\zeta w$ by

$$-\zeta w \to -\zeta(w - p\,\delta n/\overline{n}). \tag{76}$$

The generalization that subtracts out projections onto the momentum and kinetic-energy subspaces is straightforward.[35]

I have previously commented on the special status of the $(0,0)$ modes (subsequently denoted by the subscript 0). One may inquire whether addition of the basic W-stat spuriously damps those modes in realistic simulations, or conversely whether such damping may help stabilize those modes in the present slab model. Upon specializing to homogeneous simulations for simplicity, one has

$$\partial_t \delta f_0(x, \boldsymbol{v}) + \partial_x(\delta V_{E,x}\,\delta f)_0 = -C[\delta f]_0. \tag{77}$$

After taking the velocity moment, ignoring finite gyroradius effects for simplicity, and noting that the collision operator conserves number, one obtains

$$\partial_t \delta n_0(x) + \partial_x(\delta V_{E,x}\,\delta n)_0 = 0. \tag{78}$$

Here

$$(\delta V_{E,x}\,\delta n)_0(x) = \sum_{\boldsymbol{k}^\perp \neq \boldsymbol{0}} \delta V^*_{Ex,\boldsymbol{k}^\perp} \delta n_{\boldsymbol{k}^\perp}, \tag{79}$$

where $\boldsymbol{k}^\perp \equiv (k_y, k_z)$. Obviously there is no direct collisional damping on δn_0. That is described correctly if the projection (75) is used to define the W-stat.

I have noted[35] that there is some uncertainty in the proper choice of projection Q. I will now argue that the addition of a W-stat does not significantly affect the nonlinear dynamics of δn_0, even when the simplest, nonprojected W-stat (60a) is used. First rewrite Eq. (78) as

$$\partial_t \delta n_0(x,t) = -\partial_x(\delta V_{E,x}\,\delta n)_0 \equiv \widetilde{g}_0(x,t). \tag{80}$$

Note that $\widetilde{g}_0$ is functionally dependent on δn_0. The theory of Langevin representations for statistical closures[36,37,21] suggests that an adequate representation is

$$\widetilde{g}_0 = -\nu_T \delta n_0 + \widetilde{g}, \tag{81}$$

where ν_T describes coherent response and $\widetilde{g}$ is statistically independent of δn_0. In systems that achieve steady state, ν_T must be positive for linearly unstable modes; however, in general it can be negative and that appears to be the case for the present slab model. Dimensionally, $\nu_T \sim \overline{k}_x^2 D$, where $\overline{k}_x$ is a typical k_x and D, having the dimensions (although not necessarily the sign) of a cross-field diffusion coefficient, is determined by fluctuations of the short-wavelength, non-shear-flow modes.

The simplest unprojected W-stat would effectively replace ν_T by $\nu_T + \zeta$, so ζ is unimportant to the extent that $\zeta/|\nu_T| \ll 1$. This criterion can be rewritten with the aid of Eq. (65) as $(\nu_{\rm eff}\tau_{\rm ac})/(|\nu_T|\tau_{\rm ac}) \ll 1$. But in order of magnitude one expects that $|\nu_T|\tau_{\rm ac} = \mathcal{O}(1)$; hence the dynamical effects of ζ on the shear modes are unimportant for $\nu_{\rm eff}\tau_{\rm ac} \ll 1$, the same limit in which the flux has been argued to be independent of the presence of the W-stat. This is a satisfying consistency, and the conclusion is independent of the sign of ν_T. Again, this issue does not arise if the projected W-stat, Eq. (76), is used.

V. DISCUSSION

The purpose of this work is to provide a solution to the frequent criticism that fluctuation noise in collisionless δf simulations, as measured by the variance W of the marker weights, diffusively increases at long times. This behavior has been called the *entropy paradox*[3]: a statistical observable in a purported steady state is changing in time, so a true steady state has not, in fact, been achieved.

First, a rigorous derivation of the δf equation was given, paying close attention to the distinction between the background PDF f; the complete, randomly-fluctuating distribution $\widetilde{f}$; and the associated marker distributions. It was noted that not all extant algorithms implement that equation consistently. In particular, many inhomogeneous global simulations do not maintain $\langle \delta f\rangle = 0$ as they should. In principle, that problem can be cured by a systematically derived modification to the weight equation [see the $\partial_x \mathcal{G}$ term in Eq. (25)], but no attempt was made to implement that term in the present work.

Next, following the work of Ref. 3, it was pointed out that the effective collisional dissipation $\nu_{\rm eff}$ remains nonzero as the collision frequency ν is taken to zero. Strictly collisionless simulations are never correct; the limit $\nu \to 0$ is asymptotically singular. It was proposed to take $\nu_{\rm eff}$ into account by modifying the marker weight equation to include a W-stat—a time-dependent damping constructed such that W is frozen in time. This procedure deliberately violates Liouville's theorem; phase-space volumes contract in the w direction, in accord with the interpretation of the W-stat as representing the dissipative effects of the unresolved degrees of freedom. A close analogy to the thermostats of nonequilibrium molecular dynamics was noted, although the rationale for turbulent W-stats differs from that for NEMD. For NEMD, one proves that the thermostat does not change the prediction of linear response theory. For δf, one instead argues that fluxes saturate on a short autocorrelation scale whereas entropy saturates on the longer time scale of the effective dissipation, so there is a critical W above which Γ is essentially independent of W. Preliminary numerical experiments with a simple unsheared-slab model of ITG fluctuations were consistent with this prediction. This behavior leads to an extrapolation procedure wherein the time-asymptotic collisionless flux can be inferred from a series of short W-statted runs with high effective collisionality.

I considered explicitly only the Gaussian W-stat. Further consideration should be given to the relative merits of Nosé–Hoover W-stats.

The technique guarantees that entropy, a particular second-order phase-space statistical observable, is constant in time. It therefore resolves the entropy paradox by permitting a true steady state for fluxes and entropy simultaneously. No proof has been given that all other phase-space observables attain a statistical steady state as well. That is at least plausible; the dissipation introduced by the W-stat represents a qualitative improvement over the conservative Hamiltonian dynamics contained in collisionless δf, so some sort of statistical balance can be expected. However, steady states or not, it is asking too much to hope that fine-scale statistics are represented correctly by W-statted dynamics. The W-stat implements only a global phase-space constraint, in a way that eliminates long initial transients and allows for sensible, low-noise and long-time measurements of low-order fluid moments. For refined studies of phase-space structure functions and the like, one must presumably resort to detailed modelling of collisional effects, perhaps along the lines of the collisional δf algorithm of Chen and White.[6]

The method of W-statted steady states represents an attempt to be "clever" in the description of the singular limit $\nu \to 0$. As computer power increases, there will likely be a strong tendency to instead use brute force—i.e., full collisional modelling—for most simulations, including almost collisionless ones. Perhaps that is the correct approach, and it should certainly be explored. However, a general philosophy is that singular limits are dangerous, difficult, and very instructive. The work in this paper adds to one's understanding of the important singular limit $\nu \to 0$ by providing an alternative route to computing steady-state fluxes in that limit that can be used to benchmark fully collisional simulations. Such benchmarking represents an interesting goal for the future.

ACKNOWLEDGMENTS

I enjoyed early discussions on the possibility of thermostatted δf with G. Hu. I have benefitted from expert and constructively critical remarks by, and discussions with S. Brunner, Y. Chen, G. Hammett, M. Kotschenreuther, W. Lee, Z.–H. Lin, I. Manuilskiy, H. Mynick, W. Park, S. Parker, E. Valeo, and R. White.

This work was supported by U.S. Department of Energy Contract No. DE–AC02–76–CHO–3073.

APPENDIX A: ADDITIONAL REMARKS ON δf ALGORITHMS

In this section I provide some additional discussion about collisionless and collisional δf algorithms.

1. Collisionless δf and the Lagrangian phase-space lattice

It is sometimes useful to view the markers as defining the vertices of volume elements ΔA_i of a random Lagrangian phase-space lattice. For example, one might determined the ΔA's by Delaunay triangulation[38] or its generalization to higher dimensions. In collisionless theory, that lattice evolves in a simple way. To the extent that the phase-space flow is incompressible, the elementary volumes are conserved; however, generalization to compressible flow is straightforward[1] and the δf algorithm does not require that the volume elements be conserved. If the marker collision operator is negligible, and in the absence of a marker source, the effective number of marker trajectories within each elementary volume element is conserved:

$$\int_{\Delta A_i} dz\, \widehat{f}_{\mathrm{m}}(\boldsymbol{z},t) \approx \Delta A_i(t)\widetilde{f}_{\mathrm{m}}(\widetilde{\boldsymbol{z}}_i,t) \tag{A1a}$$

$$= \Delta A_i(0)\widetilde{f}_{\mathrm{m}}(\widetilde{\boldsymbol{z}}_i(0),0) \tag{A1b}$$

$$= \overline{n}_{\mathrm{m}}^{-1}. \tag{A1c}$$

Equation (A1c), which states that there is exactly one representative marker trajectory at the center of each volume element, is taken to be a precise equality, so the ΔA_i's are not uniformly distributed in space even at $t = 0$ unless $\widetilde{f}_{\mathrm{m}}(0)$ is independent of $\boldsymbol{x}$. The Eulerian moments can then be approximated as a Riemann sum[1] over the time-evolved Lagrangian lattice:

$$\delta M(\boldsymbol{z},t) = \sum_{i=1}^{N_{\mathrm{m}}} \Delta A_i(t)\widetilde{f}_{\mathrm{m}}(\overline{z},t)_{|\overline{\boldsymbol{z}}=\check{\boldsymbol{z}}_i(t)} \times \widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})w(\overline{\boldsymbol{z}},t)_{|\overline{\boldsymbol{z}}=\check{\boldsymbol{z}}_i(t)} \tag{A2a}$$

$$\approx \frac{1}{\overline{n}_{\mathrm{m}}}\sum_{i=1}^{N_{\mathrm{m}}}[\widehat{M}(\boldsymbol{z};\overline{\boldsymbol{z}})w(\overline{\boldsymbol{z}},t)]_{|\overline{\boldsymbol{z}}=\check{\boldsymbol{z}}_i(t)}. \tag{A2b}$$

This reproduces formula (20b).

This discussion provides a characterization of the way in which a collisionless sampling distribution evolves. However, it is important to stress that it is unnecessary to introduce the Lagrangian lattice or calculate the ΔA's in order to proceed with the general δf formalism. That depends only on the existence of the sampling distribution $\widetilde{g}$, which evolves in a definite way both in the presence of collisions and in their absence. For more discussion of collisional effects, see Sec. A 2.

In collisionless theory, an initial triangulation evolves smoothly and continuously, preserving positive ΔA's. In the presence of collisions (Sec. A 2), stochastic scattering can change the relative orientation of the initial vertices, making some ΔA's negative if one attempts to maintain the initial topology. However, the sampling technique does not require that a given triangulation be continuously evolved. At any time t, there always exists a triangulation with all ΔA's positive.

The Lagrangian, time-evolving phase-space lattice $\Delta A_i(t)$ should not be confused with the fixed, Eulerian spatial grid that is used to calculate discretized quantities such as $\delta\rho(\boldsymbol{x})$ in the course of solving Poisson's equation; see Fig. 8. Knowledge of the Lagrangian lattice is simply not required in order to evolve the weights. However, it may be useful in conjunction with a theory of marker sources and/or sinks. Although collisionless dynamics conserve the volume ΔA of an elementary simplex, ΔA may become highly elongated in the course of time, possibly stretching well over localized regions of important perturbations to δf. Such situations can be efficiently recognized and extra markers added to selectively improve the resolution. The inverse process of removing unnecessary markers is also possible. One possibility for such adaptive resolution involves calculation of a Delaunay triangulation, which affords one access to extensive results and computer subroutines for adaptive grid refinement in computational fluid dynamics (CFD).[39] Note that although triangulation is computationally expensive, it need be done only occasionally, not at every time step. Also, the sophisticated triangulations used in CFD enforce certain criteria that may be unnecessary for the present application. The relative merits of triangulation-based refinement vs various particle splitting schemes remain to be explored.

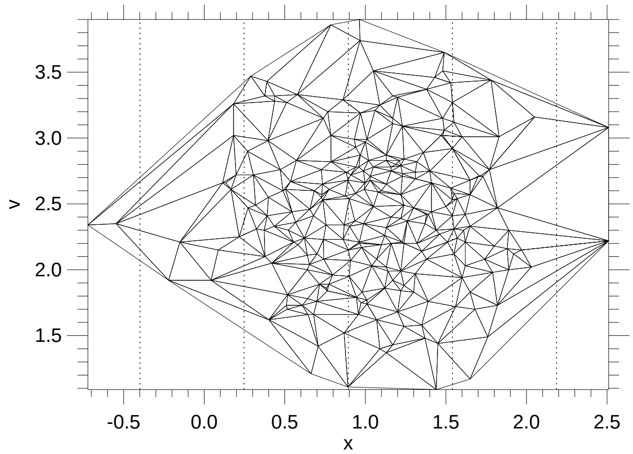

FIG. 8. The 486 triangles generated by Delaunay triangulation of an x–v phase space containing 250 points sampled from a Gaussian distribution centered around $x = 1$ and $v = 2.5$ with standard deviation $\sigma = 0.5$ in both directions. For purposes of illustration, a sample Eulerian grid represented by the dotted lines is imposed in the x direction. Calculation of potentials by Monte–Carlo sampling involves vertical sums over each bin, independent of with which triangles a point is associated. But the triangulation may be useful for adaptive refinement or coarsening of the random particle distribution.

2. Collisional δf and the algorithm of Chen and White

Recently Chen and White[6] proposed a collisional extension of the standard collisionless δf algorithm. Their procedure relied on (i) introduction of an extended $(\boldsymbol{z}, w)$ phase space; (ii) scattering the markers according to the binary-collision algorithm of Takizuka and Abe.[40] Their final results relied on the restrictive choice $\widetilde{f}_{\mathrm{m}} = \widetilde{f}$. I have already noted in general terms (Sec. II C 1) that introduction of the extended phase space is unnecessary. However, it is useful to see that more explicitly by rederiving the results of Chen and White directly from the definition (19). The discussion of this section has benefitted from an ongoing collaboration with S. Brunner and E. Valeo.

It is sufficient to focus only on binary collisions; for simplicity, I consider a single species. Thus, assume that the given dynamical equation to be solved is

$$\partial_t \widetilde{f} = -C[\widetilde{f}, \widetilde{f}], \tag{A3}$$

where C is the Landau operator, a bilinear operator that in general operates on two distinct functions a and b. Thus,

$$C[a, b] \doteq -\Gamma \frac{\partial}{\partial \boldsymbol{v}} \cdot \int d\boldsymbol{v}' \, \mathsf{U}(\boldsymbol{v} - \boldsymbol{v}') \cdot \left(\frac{\partial}{\partial \boldsymbol{v}} - \frac{\partial}{\partial \boldsymbol{v}'} \right) a(\boldsymbol{v}') b(\boldsymbol{v}), \tag{A4}$$

where $\mathsf{U}(\boldsymbol{u}) \doteq (\mathsf{I} - \widehat{u}\,\widehat{u})/u$ and Γ is proportional to the collision frequency.

Effectively, the algorithm of Takizuka and Abe simulates the Landau operator by numerically solving the random Klimontovich equation

$$\partial_t \widehat{f} + \boldsymbol{\partial}\boldsymbol{\cdot}(\widehat{\boldsymbol{a}}[\widehat{f}]\widehat{f}) = 0, \tag{A5}$$

where during any time interval Δt the random white-noise acceleration $\widehat{\boldsymbol{a}}$, functionally dependent on the statistics of the physical particles, leads to a velocity increment $\boldsymbol{\Delta v}$ that obeys Eqs. (25)–(29) of Ref. 6. Those increments are consistent with the Fokker–Planck description of small-angle velocity scattering in a plasma. That is, the fine-scaled statistical average of Eq. (A5) reduces to Eq. (A3) in the limit of small plasma parameter $\epsilon_{\mathrm{p}} \doteq 1/\overline{n}\lambda_{\mathrm{D}}^3$. Note that the fine-scaled statistical average of the generalized equation

$$\partial_t \widehat{g} = -\boldsymbol{\partial}\boldsymbol{\cdot}(\widehat{\boldsymbol{a}}[\widehat{f}]\widehat{g}) \tag{A6a}$$

is

$$\partial_t \widetilde{g} = -C[\widetilde{f}, \widetilde{g}]. \tag{A6b}$$

Now consider the reduction of Eq. (A3) to collisional δf. The procedure detailed in Sec. II B leads to

$$\begin{aligned}\partial_t \delta f &= -\{C[\widetilde{f}, \widetilde{f}] - (C[f, f] + \langle C[\delta f, \delta f]\rangle)\} \qquad &(\mathrm{A7a})\\ &= -(C[f, \delta f] + C[\delta f, f] \\ &\qquad + C[\delta f, \delta f] - \langle C[\delta f, \delta f]\rangle). &(\mathrm{A7b})\end{aligned}$$

The corresponding equation of Chen and White did not include the term $\langle C[\delta f, \delta f]\rangle$ because, following the procedures of previous workers, their definition did not include an average over macroscopic turbulent fluctuations or initial conditions, so did not satisfy $\langle \delta f\rangle = 0$.

From the definition $w \doteq \delta f/\widetilde{g}$, the evolution equation for the Eulerian field w follows directly by partial time differentation:

$$\begin{aligned}\frac{\partial w}{\partial t} &= \frac{1}{\widetilde{g}}\left(-w\frac{\partial \widetilde{g}}{\partial t} + \frac{\partial \delta f}{\partial t}\right) &(\mathrm{A8a})\\ &= \widetilde{g}^{-1}\{w\underbrace{C[\widetilde{f}, \widetilde{g}]}_{(a)} - (\underbrace{C[f, \delta f]}_{(b)} + \underbrace{C[\delta f, f]}_{(c)} \\ &\qquad + \underbrace{C[\delta f, \delta f]}_{(d)} - \underbrace{\langle C[\delta f, \delta f]\rangle}_{(e)})\}. &(\mathrm{A8b})\end{aligned}$$

Note that although this equation inherits the structure of Eq. (A7b), necessary to ensure $\langle \delta f\rangle = 0$, w does not itself have zero mean.

The goal is to find a workable equation for a stochastic $\widehat{w}$ whose fine-scaled average is w: $w = \langle \widehat{w}\rangle_{\mathrm{fine}}$. To that end, notice that because C is a bilinear operator terms (b) and (d) combine to give

$$\begin{aligned}C[\widetilde{f}, \delta f] &= C[\widetilde{f}, \langle \delta\widehat{f}\rangle_{\mathrm{fine}}] &(\mathrm{A9a})\\ &= \langle C[\widetilde{f}, \delta\widehat{f}]\rangle_{\mathrm{fine}} &(\mathrm{A9b})\\ &= \langle \boldsymbol{\partial}\boldsymbol{\cdot}(\widehat{\boldsymbol{a}}[\widehat{f}]\delta\widehat{f})\rangle_{\mathrm{fine}}, &(\mathrm{A9c})\end{aligned}$$

where $\delta\widehat{f} \doteq w\,\widehat{g}$. [The latter result strictly follows only when $\delta\widehat{f}$ obeys an equation of the form (A6a). That is not quite true due to collisional corrections represented by terms (c) and (e), but those are unimportant on the rapid time scale of the random velocity increments.] Upon recalling Eq. (A5), one then has

$$\begin{aligned}\partial_t w = \widetilde{g}^{-1}\{&w\langle \boldsymbol{\partial}\boldsymbol{\cdot}(\widehat{\boldsymbol{a}}[\widehat{f}]\widehat{g})\rangle_{\mathrm{fine}} - \langle \boldsymbol{\partial}\boldsymbol{\cdot}(\widehat{\boldsymbol{a}}[\widehat{f}]\widehat{g}w)\rangle_{\mathrm{fine}} \\ &- (C[\delta f, f] - \langle C[\delta f, \delta f]\rangle)\}. \end{aligned}\tag{A10}$$

The corresponding equation for $\widehat{w}$ is naturally defined by removing the first two averages on the right-hand side. Upon noting a partial cancellation between the $\widehat{\boldsymbol{a}}$ terms, one then finds

$$\partial_t \widehat{w} = \widetilde{g}^{-1}\{-\widehat{g}\widehat{\boldsymbol{a}}[\widehat{f}]\boldsymbol{\cdot}\boldsymbol{\partial}w - (C[\delta f, f] - \langle C[\delta f, \delta f]\rangle)\}. \tag{A11}$$

If one approximates $\widehat{g} \approx \widetilde{g}$ and $w \approx \widehat{w}$, one may take the acceleration term to the left-hand side, which becomes the total time derivative along the stochastic trajectories defined by the algorithm of Takizuka and Abe:

$$(\partial_t \widehat{w} + \widehat{\boldsymbol{a}}[\widehat{f}]\boldsymbol{\cdot}\boldsymbol{\partial}\widehat{w}) = -\widetilde{g}^{-1}(C[\delta f, f] - \langle C[\delta f, \delta f]\rangle). \tag{A12}$$

Note that here the acceleration is outside the velocity derivative; compare Eq. (A6a). Also note that the statistics of $\widehat{\boldsymbol{a}}[\widehat{f}]$ are determined by the *physical* particle distribution (including δf), not the marker distribution $\widetilde{g}$. That is problematical, since the physical δf statistics are not known (finding them is the goal of the simulation). However, following Chen and White, I note that if the marker initial conditions and source are taken to be equal to those of $\widetilde{f}$, then Eq. (A6a) is compatible with the solution $\widetilde{g} = \widetilde{f}$, and Eq. (A12) becomes, with $\widehat{f} \to \widehat{g}$,

$$(\partial_t \widehat{w} + \widehat{\boldsymbol{a}}[\widehat{g}]\boldsymbol{\cdot}\boldsymbol{\partial}\widehat{w}) \equiv \frac{d\widehat{w}}{dt} = -\widetilde{g}^{-1}(C[\delta f, f] - \langle C[\delta f, \delta f]\rangle). \tag{A13}$$

With the exception of the $\langle C[\delta f, \delta f]\rangle$ term, this is the algorithm deduced by Chen and White; see their Eq. (32).

In general, requiring $\widetilde{g} = \widetilde{f}$ is unsatisfactory because it forces one to waste resolution modelling the background f, which may be known analytically. Generalizations of the above procedure are possible in which $\widetilde{g}$ is arranged to follow more closely δf than $\widetilde{f}$. Those will be described elsewhere.

In the context of the present paper, the importance of Eq. (A13) is that it clearly shows what physics is being replaced by the thermostatting procedure. The W-stat replaces both the stochastic acceleration $\widehat{\boldsymbol{a}}[\widehat{g}]$ as well as the right-hand side of Eq. (A13). For example, the model collision operator (49) is represented entirely by $\widehat{a} = -\nu v + \delta\widehat{a}(t)$, $\delta\widehat{a}$ being Gaussian white noise with appropriate variance. For that model, the right-hand side of Eq. (A13) vanishes (for the Brownian test particle, there is no additional back-reaction of the test particle on the background in addition to the frictional drag incorporated in the $-\nu v$ term). The W-stat then provides a replacement for the time-averaged effects of $\widehat{a}$.

APPENDIX B: ENTROPY, DISSIPATION, AND THE BROWNIAN TEST PARTICLE

In this section I will use a simple Langevin–Fokker–Planck model to illustrate how the velocity-space dissipation functional (52) is in fact determined by spatial diffusion.

Consider a Brownian test ion of mass M moving in a sea of electrons of uniform temperature T. Its distribution obeys[41]

$$\frac{\partial \widetilde{f}}{\partial t} + v\frac{\partial \widetilde{f}}{\partial z} = -C[\widetilde{f}] = \nu\frac{\partial}{\partial v}\left(v + \frac{\partial}{\partial v}\right)\widetilde{f}, \tag{B1}$$

where velocities are normalized to $v_T \doteq (T/M)^{1/2}$. The steady-state solution of (B1) is a spatially uniform Maxwellian, $f(z, v) = f_{\mathrm{M}}(v)$. The fluctuation $\delta f \doteq \widetilde{f} - f$ also obeys Eq. (B1). That equation can be solved exactly for all times,[42] but it is more instructive to proceed *via* the Chapman–Enskog procedure. In Chapman–Enskog, one orders lengths to a characteristic system size L and times to the transit time L/v_T. This introduces the dimensionless parameter $\epsilon \doteq \lambda_{\mathrm{mfp}}/L \ll 1$, where $\lambda_{\mathrm{mfp}} \doteq v_T/\nu$ is the mean free path, in the denominator of the right-hand side of Eq. (B1). For macroscopic (hydrodynamic) motions, the lowest-order solution of Eq. (B1) is then $C[\delta f^{(0)}]$, or

$$\delta f^{(0)}(z, v) = \frac{\delta n(z,t)}{\overline{n}} f_{\mathrm{M}}(v), \tag{B2}$$

where δn must be determined. At first order,

$$\frac{\partial \delta f^{(0)}}{\partial t} + v\frac{\partial \delta f^{(0)}}{\partial z} = -C[\delta f^{(1)}]. \tag{B3}$$

It can be shown that density is the only quantity conserved by C, so the solvability constraint on the solution of Eq. (B3) is that the velocity integral of the left-hand side vanishes:

$$\frac{\partial}{\partial t}\left(\frac{\delta n}{\overline{n}}\right) = 0. \tag{B4}$$

This is a degenerate Euler equation that states that δn is constant on the transit time scale: $\delta n = \delta n(z, \epsilon t)$. For the first-order solution write $\delta f^{(1)} = f_{\mathrm{M}}\chi$; then the solution to $v\,\partial_z \delta f^{(0)} = -C[\delta f^{(1)}]$ can readily be shown to be

$$\chi = -\frac{v}{\nu}\frac{\partial}{\partial z}\left(\frac{\delta n}{\overline{n}}\right). \tag{B5}$$

Long-time evolution follows from the rigorous continuity equation

$$\frac{\partial}{\partial t}\left(\frac{\delta n}{\overline{n}}\right) = -\frac{\partial \Gamma}{\partial z}, \tag{B6}$$

where

$$\Gamma \doteq \int_{-\infty}^{\infty} dv\, v\, \delta f \approx \int_{-\infty}^{\infty} dv\, v\, \delta f^{(1)} = -D\frac{\partial}{\partial z}\left(\frac{\delta n}{\overline{n}}\right) \tag{B7}$$

and $D \doteq v_T^2/\nu$.

Now consider the entropy evolution from both kinetic and fluid points of view. With $w \doteq \delta f/f$, one has [cf. Eqs. (51)]

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\overline{w^2}\right) = -D_v\overline{\left(\frac{\partial w}{\partial v}\right)^2}. \tag{B8a}$$

On the other hand, from Eq. (B6) one obtains

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\overline{\left(\frac{\delta n}{\overline{n}}\right)^2}\right] = -D\overline{\left[\frac{\partial}{\partial z}\left(\frac{\delta n}{\overline{n}}\right)\right]^2}. \tag{B8b}$$

To lowest order, $w \approx w^{(0)} = \delta f^{(0)}/f = \delta n/\overline{n}$, so the left-hand sides of Eqs. (B8) are essentially equal. $w^{(0)}$ does not contribute to the right-hand side of Eq. (B8a) because $\delta n/\overline{n}$ is independent of v, but $w^{(1)} = \chi$ does. From Eq. (B5), one finds

$$\frac{\partial \chi}{\partial v} = -\frac{1}{\nu}\frac{\partial}{\partial z}\left(\frac{\delta n}{\overline{n}}\right), \tag{B9}$$

and upon substituting this result into Eq. (B8a), one consistently shows that the right-hand sides of Eqs. (B8) are equal as well. Equation (B9) is the simplest example of the link, asserted in Sec. III D, between velocity gradients and spatial gradients.

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[13] Numerical implementation of the $\partial_x \mathcal{G}$ term in the δf algorithm to be described in Sec. II C requires that $\mathcal{G}(x)$ be evaluated at the positions of the markers. This poses somewhat of a problem; although the particle and thermal fluxes are (or should be) already available as a diagnostic on the Eulerian spatial grid, direct accumulation of the full velocity-dependent $\mathcal{G}$ may be noisy and time-consuming. It may be adequate to represent δf in terms of its first few velocity-space moments, in which case $\mathcal{G}$ can be simply expressed in terms of Γ_n, Γ_T, possibly the momentum flux, and f. Splines can be used to interpolate the Γ's to all x, or it may be adequate to simply use the mapping of the x_i's onto the spatial grid; that mapping is known at each time step.
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[15] For some further remarks about random sources, see J. A. Krommes, Phys. Plasmas **4**, 1342 (1997).
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